Supplementary Information

for

High-Temperature Oxidation Chemistry of *n*-Butanol - Experiments in Low-Pressure Premixed Flames and Detailed Kinetic Modeling

by

N. Hansen, M. R. Harper, and W. H. Green

Contents:

1. Chemkin Input File The list of species (and their thermochemistry) and reactions (and their rate coefficients) that comprise the butanol mechanism

2. Transport Properties The transport properties for the species in the butanol mechanism

3. Dictionary A list of the species and their RMG-defined structure

4. Glossary A list of the species and their IUPAC International Chemical Identifiers (InChIs)

5. Temperature Profiles Experimentally measured temperature profiles for the three flames reported in this study as a function of distance from the burner

6. Thermochemical Parameters

7. Most Important Experimentally Determined Mole Fraction Profiles
please contact nhansen@sandia.gov first before use

1. Chemkin Input File:

```
!chem.inp

!UPDATED 12-MAY-2011
!GIT HASH: 94a6c93af (minus the 8d8c30ca4986ef commit)
!
!chem-PCCP-submitted.inp
!Supplementary information for manuscript:
!     "High-temperature oxidation chemistry of n-butanol - experiments
in low-pressure
!           premixed flames and detailed kinetic modeling"
!     N. Hansen, M. R. Harper, W. H. Green
!     to be submitted to: Phys. Chem. Chem. Phys.

!UPDATED 11-MAR-2011
!GIT HASH: aaff19b
!
!Sent to: N.Hansen, W.H.Green
!     on 11-MAR-2011
!     RE: Full paper on n-butanol high-temperature oxidation chemistry

!GIT HASH: b43a4bb
!N.Hansen, M.R.Harper, W.H.Green
!"High-temperature oxidation chemistry of n-butanol in low-pressure
premixed flames"
!7th U.S. National Combustion Meeting
!March 20-23, 2011, Georgia Tech, Atlanta, GA
!
!Sent to: I.Stranic, B.W.Weber, D.F.Davidson, R.K.Hanson, C.-J. Sung,
N.Hansen, W.H.Green
!     on 23-FEB-2011
!     RE: latest butanol mechanism in preparation for U.S. National
Combustion Meeting

! "Comprehensive Reaction Mechanism for n-Butanol Pyrolysis and
Combustion"
! M.R. Harper (a), K.M. Van Geem (b), G.B. Marin (b), W.H. Green (a)
! (a) Department of Chemical Engineering, Massachusetts Institute of
Technology
! (b) Laboratory for Chemical Technology, Universiteit Gent, Belgium
! Submitted to Combust. Flame

ELEMENTS
O  H  C  N  AR
END

SPECIES
H2              CO2             CO              CH4             C2H4
C2H2            C2H6            C3H6            C3H8
aC3H4
pC3H4           CH3OH           C4H8-1          C4H6-13
nC4H10
N2              C2H5OH          benzene         nC4H10O         C2H3
CH2CO           C2H4O           CH3CHO          H2O
nC4H8O
```

C4H7OJ(8)	C4H7OJ(12)	C4H7OJ(13)	C4H7OJ(16)	
CH2CHO				
C3H6O-enol2	C3H5O-enol2	CH2O	C4H8O-enol	
C4H8O-enol2				
C4H8O-enol3	C4H9O-1	C4H9O-2	C4H9O-3	
C4H9O-4				
C4H9O-5	C3H7O-N1	C3H5OJ(8)	C3H5OJ(12)	
C3H5OJ(13)				
C3H6O	C2H5	H	O	O2
OH	HO2	H2O2	C	CH
CH2	CH2(S)	CH3	HCO	
CH2OH				
CH3O	C2H	HCCO	HCCOH	AR
C2O	HOC2H4O2	C3H2	pC3H3	
aC3H5				
pC3H5	sC3H5	C3H7-1	C3H7-2	
C2H5O-1				
C2H5O-2	C2H5O-3	C3H4O-enone	C3H4O	
C4H7O-13				
C4H2	iC4H3	nC4H3	C4H4	
C4H5-113				
nC4H5	iC4H5	C4H6-1	C4H6-12	
C4H7-14				
C4H7-11	C4H7-12	C4H7-24	C4H9-1	
C4H9-2				
C2H3O-1	C2H3O-2	C6H4	C6H5	
C4H6-2				
C4H7-22	CH3CO	C6H10	C6H9_1_2_5	
C6H9_CYC_1_3				
C6H8_CYC_1_4	C6H7_CYC_1_2	C6H10_CYC	C7H9	C8H8
C8H9	C7H8	C3H7O2	CH2CH2CH2OOH	
aC3H5O2				
nSPC(301)	nSPC(351)	nSPC(385)	nSPC(447)	
nSPC(543)				
nSPC(801)	nSPC(879)	nSPC(1064)	nSPC(102)	
C4H8-2				
C3H3O-enone	FULVENE	C6H5O	C5H5	
C6H5OH				
cyC5H6	C5H5CH3_1	C5H5CH3_2	C5H5CH3_3	C8H6
C6H5CH2	C6H5CCH2	C5H4CH3	C5H5CH2-1	
C5H5CH2-2				
C5H5CH2-3	ME2CYBE	c5h4chchch2	C#CCCC#C	
C*C*CC*C*C				
CH3CCCH2	C4H4-123	C5H10_1	C5H9_1_4	
C5H8_CYC_1				
C5H9_CYC	C5H7_CYC_1_2	C4H7O_1_2	sBuOH	
CH3C[OH]C2H5				
CH3CH[OH]CHCH3	CH3CH[O]C2H5	CH2CH[OH]C2H5	CH3CH[OH]CH2CH2	
CH3CH[OH]CH2				
HOCHC2H5	H2CCCH3[OH]	CH3CH-O-CH3	CH3C[OH]CH3	
acetone				
C2H5CHCHCH2	CH2C[OH]CH2	CH2C[O]CH3	CH3-O-C(CH3)2	
C3H6O-enol				
MEK	sC4H8O	C4H6O(717)	cH2C[O]C2H5	
CH3C[O]cHCH3				

```
CH3C[O]CH2cH2    MEKenol2         CH2C[OH]cHCH3    CH2C[OH]CH2cH2
cHC[OH]C2H5
MEKenol          CH3CHcOH         CH3C[OH]cH       CH3C[OH]cCH3
CH3C[OH]CHcH2    cH2CH[OH]C2H3    CH3CH[OH]cCH2    CH3CH[OH]CHcH
CH3CH[o]C2H3
CH3CHCHCHO       CHCHCHO          CH3CCHCHO        CH3CHCHCO
C4H7O-14

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!
! New work for sec- and tert-butanol paper:
!
!    "Accurate Reaction Networks for Alternative Fuels: Butanol Isomers"
!
!    K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
!
!    To be submitted to Industrial & Engineering Chemical Research
!
!       for the ISCRE-21 conference
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!

tBuOH            iC4H8            HOC[CH2][CH3]2   OC[CH3]3
iC4H7
HCC[CH3]2        tC4H9            iC4H9            iC4H10

sSPC(116)        sSPC(46)         sSPC(56)         sSPC(752)
sSPC(332)
sSPC(1013)       sSPC(1072)       sSPC(1151)       sSPC(1356)
sSPC(1697)
sSPC(1735)       sSPC(1909)       sSPC(3071)       sSPC(3121)
sSPC(2810)
sSPC(1474)       sSPC(1590)       tSPC(54)         tSPC(77)
tSPC(122)
tSPC(157)        tSPC(213)        tSPC(97)         tSPC(439)
tSPC(343)
tSPC(346)        tSPC(878)        H2CCCO           tSPC(1286)
tSPC(1416)
tSPC(1553)       C8H14            tSPC(3683)       C4H8O2(62)
C4H7OJ(79)
tSPC(110)        C4H6O(105)       C5H10_iso        C5H9J(5)
C5H9J(7)
C5H9J(8)         C5H9J(9)         C5H11J(10)       C5H11J(11)

C5H8(95)         SPC(482)         SPC(483)         C5H7J(504)
SPC(493)
SPC(494)         SPC(495)         SPC(496)         SPC(498)
SPC(499)
C6H7J(511)       C6H7J(512)       C6H7J(505)       C6H7J(506)
C8H13J(41)
C8H15J(44)       SPC(425)         SPC(426)         C7H10(454)

C12H10
biC5H5           C5H4C5H5         C10H9            fulvalene
C10H8
```

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!!!
```

```
! NASA Polynomial format for CHEMKIN-II
! see README file for disclaimer
!O                 L 1/90O   1               G   200.000  3500.000
1000.000    1
! 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11
1.22833691E-15    2
! 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03
6.64306396E-06    3
!-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00
4
!Primary Thermo Library: CFG (Species ID: O)
O                       C   0H   0O   1     G   250.000  5000.000
995.043    1
 2.50000000E+00 1.94847979E-16-1.10543914E-19 2.31874113E-23-
1.27039788E-27    2
 2.92667023E+04 4.07323848E+00 2.50000000E+00 4.49968562E-16-
1.26455356E-18    3
 1.31186362E-21-4.54562432E-25 2.92667023E+04 4.07323848E+00
4
O2                TPIS89O   2               G   200.000  3500.000
1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-
2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03
9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00
4
H                 L 7/88H   1               G   200.000  3500.000
1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18
4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-
1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01
4
H2                TPIS78H   2               G   200.000  3500.000
1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10
2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-
1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01
4
!OH                RUS 78O   1H   1          G   200.000  3500.000
1000.000    1
! 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11
1.17412376E-14    2
! 3.85865700E+03 4.47669610E+00 3.99201543E+00-2.40131752E-03
4.61793841E-06    3
!-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01
4
!Primary Thermo Library: CFG (Species ID: OH)
OH                      C   0H   1O   1     G   250.000  5000.000
995.043    1
 3.05213635E+00 6.84823853E-04-8.07335807E-08-3.71699421E-12
8.83223831E-16    2
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 3.48176639E+03 3.92578182E+00 3.46140051E+00 3.67265808E-04-
1.60342624E-06    3
 2.35738448E-09-9.29231871E-13 3.33459312E+03 1.62308450E+00
4
H2O               L 8/89H   2O   1          G   200.000  3500.000
1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11
1.68200992E-14    2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03
6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01
4
HO2               L 5/89H   1O   2          G   200.000  3500.000
1000.000    1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-
1.07908535E-14    2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03
2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00
4
H2O2              L 7/88H   2O   2          G   200.000  3500.000
1000.000    1
 4.16500285E+00 4.90831694E-03-1.90139225E-06 3.71185986E-10-
2.87908305E-14    2
-1.78617877E+04 2.91615662E+00 4.27611269E+00-5.42822417E-04
1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77025821E+04 3.43505074E+00
4
C                 L11/88C   1          G   200.000  3500.000
1000.000    1
 2.49266888E+00 4.79889284E-05-7.24335020E-08 3.74291029E-11-
4.87277893E-15    2
 8.54512953E+04 4.80150373E+00 2.55423955E+00-3.21537724E-04
7.33792245E-07    3
-7.32234889E-10 2.66521446E-13 8.54438832E+04 4.53130848E+00
4
CH                TPIS79C   1H   1          G   200.000  3500.000
1000.000    1
 2.87846473E+00 9.70913681E-04 1.44445655E-07-1.30687849E-10
1.76079383E-14    2
 7.10124364E+04 5.48497999E+00 3.48981665E+00 3.23835541E-04-
1.68899065E-06    3
 3.16217327E-09-1.40609067E-12 7.07972934E+04 2.08401108E+00
4
CH2               L S/93C   1H   2          G   200.000  3500.000
1000.000    1
 2.87410113E+00 3.65639292E-03-1.40894597E-06 2.60179549E-10-
1.87727567E-14    2
 4.62636040E+04 6.17119324E+00 3.76267867E+00 9.68872143E-04
2.79489841E-06    3
-3.85091153E-09 1.68741719E-12 4.60040401E+04 1.56253185E+00
4
CH2(S)            L S/93C   1H   2          G   200.000  3500.000
1000.000    1
 2.29203842E+00 4.65588637E-03-2.01191947E-06 4.17906000E-10-
3.39716365E-14    2
```

```
 5.09259997E+04 8.62650169E+00 4.19860411E+00-2.36661419E-03
8.23296220E-06    3
-6.68815981E-09 1.94314737E-12 5.04968163E+04-7.69118967E-01
4

!Primary Thermo Library: Burcat (Species ID: CH3)
CH3                     C   1H   3          G   300.000  5000.000
995.043    1
 3.30135733E+00 5.18030141E-03-1.62114306E-06 2.37831978E-10-
1.33298751E-14    2
 1.63968951E+04 2.94688270E+00 3.96853937E+00-8.71548811E-05
1.02168742E-05    3
-1.03047546E-08 3.29151406E-12 1.63921134E+04 3.74584663E-01
4
!CH3                L11/89C   1H   3          G   200.000  3500.000
1000.000    1
! 2.28571772E+00 7.23990037E-03-2.98714348E-06 5.95684644E-10-
4.67154394E-14    2
! 1.67755843E+04 8.48007179E+00 3.67359040E+00 2.01095175E-03
5.73021856E-06    3
!-6.87117425E-09 2.54385734E-12 1.64449988E+04 1.60456433E+00
4

CH4                L 8/88C   1H   4          G   200.000  3500.000
1000.000    1
 7.48514950E-02 1.33909467E-02-5.73285809E-06 1.22292535E-09-
1.01815230E-13    2
-9.46834459E+03 1.84373180E+01 5.14987613E+00-1.36709788E-02
4.91800599E-05    3
-4.84743026E-08 1.66693956E-11-1.02466476E+04-4.64130376E+00
4
CO                 TPIS79C   1O   1          G   200.000  3500.000
1000.000    1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-
2.03647716E-14    2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04
1.01681433E-06    3
 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00
4
CO2                L 7/88C   1O   2          G   200.000  3500.000
1000.000    1
 3.85746029E+00 4.41437026E-03-2.21481404E-06 5.23490188E-10-
4.72084164E-14    2
-4.87591660E+04 2.27163806E+00 2.35677352E+00 8.98459677E-03-
7.12356269E-06    3
 2.45919022E-09-1.43699548E-13-4.83719697E+04 9.90105222E+00
4
HCO                L12/89H   1C   1O   1     G   200.000  3500.000
1000.000    1
 2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-
5.33508711E-14    2
 4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03
1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00
4
CH2O               L 8/88H   2C   1O   1     G   200.000  3500.000
1000.000    1
```

```
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-
8.83855640E-14    2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03
3.73220008E-05    3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01
4

!Burcat
CH2OH RADICAL     IU2/03C  1.H  3.O  1.   0.G   200.000  6000.000 1000.
1
 5.09312037E+00 5.94758550E-03-2.06496524E-06 3.23006703E-10-
1.88125052E-14    2
-4.05813228E+03-1.84690613E+00 4.47832317E+00-1.35069687E-03
2.78483707E-05    3
-3.64867397E-08 1.47906775E-11-3.52476728E+03 3.30911984E+00-
2.06867272E+03    4
!CH2OH             GUNL93C   1H   3O   1     G   200.000  3500.000
1000.000    1
! 3.69266569E+00 8.64576797E-03-3.75101120E-06 7.87234636E-10-
6.48554201E-14    2
!-3.24250627E+03 5.81043215E+00 3.86388918E+00 5.59672304E-03
5.93271791E-06    3
!-1.04532012E-08 4.36967278E-12-3.19391367E+03 5.47302243E+00
4

!Burcat
CH3O  METHOXY RAD IU1/03C  1.H  3.O  1.   0.G   200.000  6000.000 1000.
1
 4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-
2.63537098E-14    2
 3.90139164E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03
3.76550971E-05    3
-4.73072089E-08 1.86588420E-11 1.30772484E+03 6.57240864E+00
2.53773223E+03    4
!CH3O              121686C   1H   3O   1     G   300.00   3000.00
1000.000    1
! 0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-
0.02112616E-12    2
! 0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01
0.05338472E-04    3
!-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02
4

CH3OH             L 8/88C   1H   4O   1     G   200.000  3500.000
1000.000    1
 1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-
1.17060220E-13    2
-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02
6.52441155E-05    3
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00
4
C2H               L 1/91C   2H   1          G   200.000  3500.000
1000.000    1
 3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-
1.77232770E-14    2
 6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-
2.84769501E-05    3
```

```
 2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00
4
C2H2              L 1/91C   2H   2          G   200.000  3500.000
1000.000    1
 4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-
3.61235213E-14    2
 2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-
3.55171815E-05    3
 2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01
4
C2H3              L 2/92C   2H   3          G   200.000  3500.000
1000.000    1
 3.01672400E+00 1.03302292E-02-4.68082349E-06 1.01763288E-09-
8.62607041E-14    2
 3.46128739E+04 7.78732378E+00 3.21246645E+00 1.51479162E-03
2.59209412E-05    3
-3.57657847E-08 1.47150873E-11 3.48598468E+04 8.51054025E+00
4
C2H4              L 1/91C   2H   4          G   200.000  3500.000
1000.000    1
 2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-
1.25706061E-13    2
 4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03
5.70990292E-05    3
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00
4

!Burcat
C2H5 ethyl radic  IU1/07C  2.H  5.   0.   0.G   200.000  6000.000 1000.
1
 4.32195633E+00 1.23930542E-02-4.39680960E-06 7.03519917E-10-
4.18435239E-14    2
 1.21759475E+04 1.71103809E-01 4.24185905E+00-3.56905235E-03
4.82667202E-05    3
-5.85401009E-08 2.25804514E-11 1.29690344E+04 4.44703782E+00
1.43965189E+04    4
!C2H5              L12/92C   2H   5          G   200.000  3500.000
1000.000    1
! 1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-
1.49641576E-13    2
! 1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03
4.97142807E-05    3
!-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00
4

C2H6              L 8/88C   2H   6          G   200.000  3500.000
1000.000    1
 1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-
1.90002890E-13    2
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03
5.99438288E-05    3
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00
4
CH2CO             L 5/90C   2H   2O   1     G   200.000  3500.000
1000.000    1
 4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-
7.94838201E-14    2
```

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-7.55105311E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-
1.73947474E-05    3
 9.34397568E-09-2.01457615E-12-7.04291804E+03 1.22156480E+01
4
HCCO              SRIC91H   1C   2O   1     G   300.00   4000.00
1000.000    1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-
0.19407832E-13    2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-
0.23729101E-04    3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02
4
HCCOH              SRI91C   2O   1H   2     G   300.000  5000.000
1000.000    1
 0.59238291E+01 0.67923600E-02-0.25658564E-05 0.44987841E-09-
0.29940101E-13    2
 0.72646260E+04-0.76017742E+01 0.12423733E+01 0.31072201E-01-
0.50866864E-04    3
 0.43137131E-07-0.14014594E-10 0.80316143E+04 0.13874319E+02
4
H2CN               41687H   2C   1N   1     G   300.00   4000.000
1000.000    1
 0.52097030E+01 0.29692911E-02-0.28555891E-06-0.16355500E-09
0.30432589E-13    2
 0.27677109E+05-0.44444780E+01 0.28516610E+01 0.56952331E-02
0.10711400E-05    3
-0.16226120E-08-0.23511081E-12 0.28637820E+05 0.89927511E+01
4
HCN               GRI/98H   1C   1N   1     G   200.000  6000.000
1000.000    1
 0.38022392E+01 0.31464228E-02-0.10632185E-05 0.16619757E-09-
0.97997570E-14    2
 0.14407292E+05 0.15754601E+01 0.22589886E+01 0.10051170E-01-
0.13351763E-04    3
 0.10092349E-07-0.30089028E-11 0.14712633E+05 0.89164419E+01
4
HNO               And93 H   1N   1O   1     G   200.000  6000.000
1000.000    1
 0.29792509E+01 0.34944059E-02-0.78549778E-06 0.57479594E-10-
0.19335916E-15    2
 0.11750582E+05 0.86063728E+01 0.45334916E+01-0.56696171E-02
0.18473207E-04    3
-0.17137094E-07 0.55454573E-11 0.11548297E+05 0.17498417E+01
4
N                 L 6/88N   1               G   200.000  6000.000
1000.000    1
 0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226245E-10-
0.20360982E-14    2
 0.56133773E+05 0.46496096E+01 0.25000000E+01 0.00000000E+00
0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.56104637E+05 0.41939087E+01
4
NNH               T07/93N   2H   1          G   200.000  6000.000
1000.000    1
 0.37667544E+01 0.28915082E-02-0.10416620E-05 0.16842594E-09-
0.10091896E-13    2
```

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 0.28650697E+05 0.44705067E+01 0.43446927E+01-0.48497072E-02
0.20059459E-04    3
-0.21726464E-07 0.79469539E-11 0.28791973E+05 0.29779410E+01
4
N2O               L 7/88N   2O   1          G   200.000  6000.000
1000.000    1
 0.48230729E+01 0.26270251E-02-0.95850874E-06 0.16000712E-09-
0.97752303E-14    2
 0.80734048E+04-0.22017207E+01 0.22571502E+01 0.11304728E-01-
0.13671319E-04    3
 0.96819806E-08-0.29307182E-11 0.87417744E+04 0.10757992E+02
4
NH                And94 N   1H   1          G   200.000  6000.000
1000.000    1
 0.27836928E+01 0.13298430E-02-0.42478047E-06 0.78348501E-10-
0.55044470E-14    2
 0.42120848E+05 0.57407799E+01 0.34929085E+01 0.31179198E-03-
0.14890484E-05    3
 0.24816442E-08-0.10356967E-11 0.41880629E+05 0.18483278E+01
4
NH2               And89 N   1H   2          G   200.000  6000.000
1000.000    1
 0.28347421E+01 0.32073082E-02-0.93390804E-06 0.13702953E-09-
0.79206144E-14    2
 0.22171957E+05 0.65204163E+01 0.42040029E+01-0.21061385E-02
0.71068348E-05    3
-0.56115197E-08 0.16440717E-11 0.21885910E+05-0.14184248E+00
4
NH3               J 6/77N   1H   3          G   200.000  6000.000
1000.000    1
 0.26344521E+01 0.56662560E-02-0.17278676E-05 0.23867161E-09-
0.12578786E-13    2
-0.65446958E+04 0.65662928E+01 0.42860274E+01-0.46605230E-02
0.21718513E-04    3
-0.22808887E-07 0.82638046E-11-0.67417285E+04-0.62537277E+00
4
NO                RUS 78N   1O   1          G   200.000  6000.000
1000.000    1
 0.32606056E+01 0.11911043E-02-0.42917048E-06 0.69457669E-10-
0.40336099E-14    2
 0.99209746E+04 0.63693027E+01 0.42184763E+01-0.46389760E-02
0.11041022E-04    3
-0.93361354E-08 0.28035770E-11 0.98446230E+04 0.22808464E+01
4
NO2               L 7/88N   1O   2          G   200.000  6000.000
1000.000    1
 0.48847542E+01 0.21723956E-02-0.82806906E-06 0.15747510E-09-
0.10510895E-13    2
 0.23164983E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02
0.16657812E-04    3
-0.20475426E-07 0.78350564E-11 0.28966179E+04 0.63119917E+01
4
HCNO              BDEA94H   1N   1C   1O   1G   300.000  5000.000
1382.000    1
 6.59860456E+00 3.02778626E-03-1.07704346E-06 1.71666528E-10-
1.01439391E-14    2
```

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 1.79661339E+04-1.03306599E+01 2.64727989E+00 1.27505342E-02-
1.04794236E-05    3
 4.41432836E-09-7.57521466E-13 1.92990252E+04 1.07332972E+01
4
HOCN              BDEA94H   1N   1C   1O   1G   300.000  5000.000
1368.000    1
 5.89784885E+00 3.16789393E-03-1.11801064E-06 1.77243144E-10-
1.04339177E-14    2
-3.70653331E+03-6.18167825E+00 3.78604952E+00 6.88667922E-03-
3.21487864E-06    3
 5.17195767E-10 1.19360788E-14-2.82698400E+03 5.63292162E+00
4
HNCO              BDEA94H   1N   1C   1O   1G   300.000  5000.000
1478.000    1
 6.22395134E+00 3.17864004E-03-1.09378755E-06 1.70735163E-10-
9.95021955E-15    2
-1.66599344E+04-8.38224741E+00 3.63096317E+00 7.30282357E-03-
2.28050003E-06    3
-6.61271298E-10 3.62235752E-13-1.55873636E+04 6.19457727E+00
4
NCO               EA 93 N   1C   1O   1     G   200.000  6000.000
1000.000    1
 0.51521845E+01 0.23051761E-02-0.88033153E-06 0.14789098E-09-
0.90977996E-14    2
 0.14004123E+05-0.25442660E+01 0.28269308E+01 0.88051688E-02-
0.83866134E-05    3
 0.48016964E-08-0.13313595E-11 0.14682477E+05 0.95504646E+01
4
CN                HBH92 C   1N   1          G   200.000  6000.000
1000.000    1
 0.37459805E+01 0.43450775E-04 0.29705984E-06-0.68651806E-10
0.44134173E-14    2
 0.51536188E+05 0.27867601E+01 0.36129351E+01-0.95551327E-03
0.21442977E-05    3
-0.31516323E-09-0.46430356E-12 0.51708340E+05 0.39804995E+01
4
HCNN              SRI/94C   1N   2H   1     G   300.000  5000.000
1000.000    1
 0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-
0.20094686E-13    2
 0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-
0.18816354E-04    3
 0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02
4
N2                121286N   2              G   300.000  5000.000
1000.000    1
 0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-
0.06753351E-13    2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-
0.03963222E-04    3
 0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02
4
AR                120186AR  1              G   300.000  5000.000
1000.000    1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.00000000E+00    2
```

```
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00
0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02
4
C3H8              L 4/85C   3H   8          G   300.000  5000.000
1000.000    1
 0.75341368E+01 0.18872239E-01-0.62718491E-05 0.91475649E-09-
0.47838069E-13    2
-0.16467516E+05-0.17892349E+02 0.93355381E+00 0.26424579E-01
0.61059727E-05    3
-0.21977499E-07 0.95149253E-11-0.13958520E+05 0.19201691E+02
4
! DO NOT WANT TO USE GRI-MECH DEFINED C3H7 SPECIES
!C3H7              L 9/84C   3H   7          G   300.000  5000.000
1000.000    1
! 0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-
0.39392284E-13    2
! 0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01
0.23800540E-05    3
!-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02
4
CH3CHO            L 8/88C   2H   4O   1     G   200.000  6000.000
1000.000    1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-
0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02
0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01
4
CH2CHO            SAND86O   1H   3C   2     G   300.000  5000.000
1000.000    1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-
0.02176017E-12    2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01
0.01891492E-04    3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02
4

! The following are from the Marinov mechanism
C2O               121286C   2O   1          g  0300.00   5000.00
1000.00      1
 0.04849809e+02 0.02947585e-01-0.01090729e-04 0.01792562e-08-
0.01115758e-12    2
 0.03282055e+06-0.06453226e+01 0.03368851e+02 0.08241803e-01-
0.08765145e-04    3
 0.05569262e-07-0.01540009e-10 0.03317081e+06 0.06713314e+02
4
!sC3H5              82489C   3H   5          g  0300.00   4000.00
1000.00      1
! 0.09101018e+02 0.07964168e-01-0.07884945e-05-0.04562036e-08
0.08529212e-12    2
! 0.02670680e+06-0.02150559e+03 0.03385811e+02 0.01404534e+00
0.03204127e-04    3
!-0.03824120e-07-0.09053742e-11 0.02909066e+06 0.01126649e+03
4
!sC3H5  CH3C*=CH2  T 6/96C   3H   5    0    0G   200.000  6000.000 1000.
1
```

```
! 0.61101805E+01 0.14673395E-01-0.53676822E-05 0.86904932E-09-
0.51932006E-13    2
! 0.25532442E+05-0.83555712E+01 0.25544033E+01 0.10986798E-01
0.30174305E-04    3
!-0.47253568E-07 0.19771073E-10 0.27150242E+05 0.13207592E+02
0.28582707E+05    4
!Primary Thermo Library: Franklin (Species ID: propen1yl)
sC3H5                   C   3H   5          G   300.000  5000.000
995.043    1
 6.16015254E+00 1.32220376E-02-4.59616888E-06 7.28285694E-10-
4.31606069E-14    2
 2.82933722E+04-7.09085113E+00 3.85096272E+00 6.32881309E-03
3.01800623E-05    3
-3.89089471E-08 1.40202574E-11 2.95537218E+04 8.06213245E+00
4
!HCOH              mar94 C   1H   2O   1    0g   300.     5000.    1398.
1
! 9.18749272e+00 1.52011152e-03-6.27603516e-07 1.09727989e-10-
6.89655128e-15    2
! 7.81364593e+03-2.73434214e+01-2.82157421e+00 3.57331702e-02-
3.80861580e-05    3
! 1.86205951e-08-3.45957838e-12 1.12956672e+04 3.48487757e+01
4
HCOOH             103190C   1H   2O   2     g  0300.00   4000.00
1500.00      1
 0.07959698E+02 0.03024532E-01-0.03434242E-05-0.01326767E-08
0.02520240E-12    2
-0.05027445E+06-0.01872208E+03 0.09326031E+01 0.01891002E+00-
0.01554964E-03    3
 0.07290031E-07-0.01483695E-10-0.04760071E+06 0.01950653E+03
4
C2H5OH                  C   2H   6O   1    0g   300.000  5000.000
1000.000     1
 0.65624365e+01 0.15204222e-01-0.53896795e-05 0.86225011e-09-
0.51289787e-13    2
-0.31525621e+05-0.94730202e+01 0.48586957e+01-0.37401726e-02
0.69555378e-04    3
-0.88654796e-07 0.35168835e-10-0.29996132e+05 0.48018545e+01
4
C2H5O-3                 C   2H   5O   1     g  0300.00   5000.00
1405.00      1
 8.31182392e+00 1.03426319e-02-3.39186089e-06 5.12212617e-10-
2.91601713e-14    2
-6.13097954e+03-2.13985581e+01-2.71296378e-01 2.98839812e-02-
1.97090548e-05    3
 6.37339893e-09-7.77965054e-13-3.16397196e+03 2.47706003e+01
4
CH3CO                   C   2H   3O   1     g  0300.00   5000.00
1000.00      1
 0.05612279e+02 0.08449886e-01-0.02854147e-04 0.04238376e-08-
0.02268404e-12    2
-0.05187863e+05-0.03274949e+02 0.03125278e+02 0.09778220e-01
0.04521448e-04    3
-0.09009462e-07 0.03193718e-10-0.04108508e+05 0.01122885e+03
4
HOC2H4O2                C   2H   5O   3    0g   300.000  5000.
1395.00      1
```

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 9.22339915e+00 1.41346358e-02-4.75283025e-06 7.28795964e-10-
4.18969629e-14    2
-2.35984031e+04-1.53847386e+01 3.58811609e+00 2.99414161e-02-
2.35156549e-05    3
 1.12635525e-08-2.28663686e-12-2.17409435e+04 1.42166729e+01
4
HCOCHO                  C   2H   2O   2    0g   300.     5000.    1396.
1
 9.75438561e+00 4.97645947e-03-1.74410483e-06 2.75586994e-10-
1.61969892e-14    2
-2.95832896e+04-2.48038370e+01 1.88105121e+00 2.36386368e-02-
1.83443295e-05    3
 6.84842963e-09-9.92733674e-13-2.69280190e+04 1.72994753e+01
4
C3H7-2                  C   3H   7    0    0g   300.     5000.    1373.
1
 9.73563939e+00 1.43303634e-02-4.88106037e-06 7.56304810e-10-
4.38380156e-14    2
 5.67000911e+03-2.78414926e+01 5.86358461e-01 3.21021065e-02-
1.69517004e-05    3
 3.98986301e-09-2.87510333e-13 9.26003586e+03 2.26632577e+01
4
pC3H5                   C   3H   5          g  0300.00   4000.00
1000.00      1
 0.09209764e+02 0.07871413e-01-0.07724523e-05-0.04497357e-08
0.08377272e-12    2
 0.02853967e+06-0.02232370e+03 0.03161863e+02 0.01518100e+00
0.02722659e-04    3
-0.05177112e-07 0.05435286e-12 0.03095548e+06 0.01197973e+03
4
C3H4O-enone             C   3H   4O   1    0g   300.00   5000.    1392.
1
 9.40386796e+00 9.90994860e-03-3.34130605e-06 5.13787016e-10-
2.96102254e-14    2
-1.42771281e+04-2.42902025e+01 2.69187311e+00 2.49761396e-02-
1.61712107e-05    3
 5.46391115e-09-7.62496644e-13-1.18758805e+04 1.19898101e+01
4
!Primary Thermo Library: Franklin (Species ID: CH2CHCO)
C3H3O-enone             C   3H   3O   1     G   300.000  5000.000
995.043    1
 7.83073435E+00 9.66335269E-03-3.36730191E-06 5.31896024E-10-
3.14004124E-14    2
 9.01866337E+03-1.45493229E+01 3.71354715E+00 9.15554897E-03
2.31135729E-05    3
-3.44389619E-08 1.30835757E-11 1.06825134E+04 9.53677358E+00
4
C3H5O-enal              C   3H   5O   1    0g   300.000  5000.000
1000.00      1
 9.44477437e+00 1.27039625e-02-4.56349179e-06 8.06113328e-10-
5.26599798e-14    2
 6.70242803e+03-2.49387079e+01-2.08814829e-03 3.58473202e-02-
2.67606354e-05    3
 1.06914296e-08-1.76330732e-12 9.89673084e+03 2.54501512e+01
4

! The following were added for n-butanol chemistry, as computed by RMG
```

```
! Note: all ATcT data are as of 05/27/2008
! ftp://ftp.technion.ac.il/pub/supported/aetdd/thermodynamics/THERM.DAT

C3H2 RMG               C   3H   2O   0     G   300.000  5000.000
995.043    1
 5.23659121E+00 7.17558058E-03-1.79402607E-06 1.62979516E-10-
4.00857498E-15    2
 5.88323643E+04-2.48721668E-01 3.19920491E+00 1.06184960E-02
1.72192871E-07    3
-5.94901202E-09 2.73623544E-12 5.94728356E+04 1.07512889E+01
4
!C3H2 ATcT              C  3.H  2.   0.   0.G   200.000  6000.000 1000.
1
! 7.47247827E+00 4.57765160E-03-1.56482125E-06 2.43991965E-10-
1.42462924E-14    2
! 8.83321441E+04-1.27113314E+01 3.74356467E+00 2.51955211E-02-
4.62608277E-05    3
! 4.34360520E-08-1.53992558E-11 8.89297787E+04 4.22612394E+00
9.08356403E+04    4

!pC3H3 RMG              C   3H   3O   0     G   300.000  5000.000
995.043    1
! 6.09017276E+00 9.08825474E-03-3.34402914E-06 5.09016554E-10-
2.86908485E-14    2
! 3.84826145E+04-8.18254441E+00 3.60098848E+00 7.42708673E-03
1.67485896E-05    3
!-2.47368473E-08 9.27490802E-12 3.95555894E+04 6.71637833E+00
4
!pC3H3 ATcT             C   3H   3    0    0G   200.000  6000.000 1000.
1
! 7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-
2.51475415E-14    2
! 3.89087427E+04-1.25848435E+01 1.35110927E+00 3.27411223E-02-
4.73827135E-05    3
! 3.76309808E-08-1.18540923E-11 4.01057783E+04 1.52058924E+01
4.16139977E+04    4
!Primary Thermo Library: Franklin (Species ID: C3H3)
pC3H3                  C   3H   3          G   300.000  5000.000
995.043    1
 7.52141010E+00 6.49532827E-03-1.96121786E-06 2.78061412E-10-
1.51245167E-14    2
 4.04743871E+04-1.51280254E+01 3.60683149E+00 1.22049797E-02
4.54657273E-06    3
-1.42089043E-08 6.16897899E-12 4.17497971E+04 6.23234158E+00
4


!pC3H4 RMG         101993H   4C   3          g   300.00   4000.00
1400.00      1
! 6.49915743E+00 1.03333141E-02-3.44377558E-06 5.31758469E-10-
3.09746438E-14    2
! 1.95733009E+04-1.12322911E+01 3.23861443E+00 1.03401230E-02
1.62943646E-05    3
!-2.59237505E-08 9.94012980E-12 2.08707158E+04 7.74058985E+00
4
pC3H4 ATcT             H   4C   3    0    0G   200.000  6000.000 1000.
1
```

```
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-
0.38299635E-13    2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01
0.25070596E-05    3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01
0.22302059E+05    4

aC3H4 RMG               C   3H   4O   0     G   300.000  5000.000
995.043    1
 6.20209785E+00 1.16035113E-02-4.24253157E-06 6.49613596E-10-
3.68734350E-14    2
 2.06143760E+04-9.81677751E+00 3.56619360E+00 4.29172814E-03
3.37754983E-05    3
-4.29088118E-08 1.54512117E-11 2.20254845E+04 7.34162599E+00
4
!aC3H4 ATcT              C   3H   4    0    0G   200.000  6000.000 1000.
1
! 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-
0.37875540E-13    2
! 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01
0.18539880E-04    3
!-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02
0.22962267E+05    4

aC3H5 RMG               C   3H   5O   0     G   300.000  5000.000
995.043    1
 6.96109932E+00 1.34091360E-02-4.82564565E-06 7.27992496E-10-
4.07881357E-14    2
 1.71186562E+04-1.40191478E+01 3.41167769E+00 2.34104588E-03
5.00532991E-05    3
-6.16298250E-08 2.20555994E-11 1.90793181E+04 9.38984818E+00
4
!aC3H5 ATcT              C   3H   5    0    0G   200.000  6000.000 1000.
1
! 0.70094568E+01 0.13106629E-01-0.46533442E-05 0.74514323E-09-
0.44350051E-13    2
! 0.16412909E+05-0.13946114E+02 0.14698036E+01 0.19034365E-01
0.14480425E-04    3
!-0.35468652E-07 0.16647594E-10 0.18325831E+05 0.16724114E+02
0.19675772E+05    4

C3H6 RMG                C   3H   6O   0     G   300.000  5000.000
995.043    1
 5.42559783E+00 1.75791067E-02-6.56311899E-06 1.03199697E-09-
5.99721148E-14    2
-6.08798934E+02-5.16515272E+00 3.64255985E+00 3.89757558E-03
4.54910439E-05    3
-5.49011352E-08 1.92835688E-11 7.78191818E+02 8.61457909E+00
4
!C3H6 ATcT               C  3.H  6.   0.   0.G   200.000  6000.000 1000.
1
! 6.03870234E+00 1.62963931E-02-5.82130800E-06 9.35936829E-10-
5.58603143E-14    2
!-7.41715057E+02-8.43825992E+00 3.83464468E+00 3.29078952E-03
5.05228001E-05    3
!-6.66251176E-08 2.63707473E-11 7.88717123E+02 7.53408013E+00
2.40543339E+03    4
```

```
!C3H7-1 RMG         mar97C   3H   7    0    0g   300.     5000.    1390.
1
! 9.43799350e 00 1.47160681e-02-5.03338420e-06 7.81317497e-10-
4.35209260e-14    2
! 7.27396508e 03-2.60136738e 01 1.13366571e-01 3.54171389e-02-
2.28073697e-05    3
! 7.88746806e-09-1.16856961e-12 1.06821595e 04 2.45520758e 01
4
C3H7-1 ATcT             C  3.H  7.   0.   0.G   200.000  6000.000 1000.
1
 6.49636579E+00 1.77337992E-02-6.24898046E-06 9.95389495E-10-
5.90199770E-14    2
 8.85973885E+03-8.56389710E+00 4.08211458E+00 5.23240341E-03
5.13554466E-05    3
-6.99343598E-08 2.81819493E-11 1.04074558E+04 8.39534919E+00
1.21859256E+04    4

!C4H2 RMG                C   4H   2O   0     G   300.000  5000.000
995.043    1
! 9.37421267E+00 5.20349912E-03-1.47494871E-06 1.97502945E-10-
1.02254888E-14    2
! 4.94560974E+04-2.49964595E+01 2.93118262E+00 2.52824972E-02-
2.29677151E-05    3
! 8.71773148E-09-6.73654919E-13 5.10265126E+04 7.50358165E+00
4
C4H2 ATcT               C  4.H  2.   0.   0.G   200.000  6000.000 1000.
1
 8.68978130E+00 6.69732229E-03-2.34774865E-06 3.72759231E-10-
2.20554548E-14    2
 5.19942624E+04-2.20010465E+01-5.84768273E-01 5.33506727E-02-
9.50805952E-05    3
 8.37959674E-08-2.80912179E-11 5.36111160E+04 2.09878997E+01
5.51203407E+04    4

iC4H3 RMG               C   4H   3O   0     G   300.000  5000.000
995.043    1
 7.77440397E+00 1.05572059E-02-3.57579563E-06 5.05608808E-10-
2.67045971E-14    2
 5.62075473E+04-1.38057490E+01 3.26868663E+00 1.85571875E-02-
3.90966010E-07    3
-1.18418769E-08 5.64168836E-12 5.76048567E+04 1.04249776E+01
4
!C4H3 ATcT               C  4.H  3.   0.   0.G   200.000  6000.000 1000.
1
! 8.44631306E+00 9.07291526E-03-3.18681201E-06 5.06725048E-10-
3.00149855E-14    2
! 6.20007365E+04-1.77938854E+01 5.54263934E-01 3.86185425E-02-
4.70818280E-05    3
! 3.06240321E-08-7.90588421E-12 6.37974910E+04 2.10542043E+01
6.53200393E+04    4

nC4H3 rmg               C   4H   3O   0     G   300.000  5000.000
995.043    1
 9.80207689E+00 8.16428021E-03-3.00989858E-06 4.48881808E-10-
2.47165121E-14    2
```

```
 5.98913234E+04-2.64748589E+01 3.28144591E+00 1.37795061E-02
1.95750799E-05    3
-3.54857594E-08 1.42303538E-11 6.22086615E+04 1.00747952E+01
4

!C4H4 RMG                C   4H   4O   0     G   300.000  5000.000
995.043    1
! 9.53726854E+00 1.11114691E-02-4.09447607E-06 6.20848240E-10-
3.48104088E-14    2
! 3.01377145E+04-2.67780310E+01 3.27449293E+00 1.07223742E-02
3.50306178E-05    3
!-5.14128529E-08 1.95256705E-11 3.26496687E+04 9.76468497E+00
4
C4H4 ATcT               C  4.H  4.   0.   0.G   200.000  6000.000 1000.
1
 7.98456038E+00 1.20558816E-02-4.23587475E-06 6.73646140E-10-
3.99059864E-14    2
 3.11993029E+04-1.67958975E+01 1.37368786E+00 2.88801256E-02-
1.46863874E-05    3
-3.91045446E-09 4.78133572E-12 3.30633344E+04 1.75941274E+01
3.46213066E+04    4

C4H5 RMG                C   4H   5O   0     G   300.000  5000.000
995.043    1
 6.49266056E+00 1.68368773E-02-5.45924754E-06 7.50059603E-10-
3.86696159E-14    2
 3.43960771E+04-7.96071084E+00 3.03787313E+00 1.96385363E-02
7.02967924E-06    3
-1.88144450E-08 7.69003801E-12 3.56324440E+04 1.14473175E+01
4
!C4H5 ATcT               C  4.H  5.   0.   0.G   200.000  6000.000 1000.
1
! 9.21572256E+00 1.34939872E-02-4.82517726E-06 7.76676426E-10-
4.64039105E-14    2
! 3.43129071E+04-2.25232815E+01 2.15189267E+00 3.05033422E-02-
1.64053256E-05    3
!-1.54978415E-11 2.38039347E-12 3.64447930E+04 1.47100046E+01
3.82983108E+04    4

C4H6-12 RMG             C   4H   6O   0     G   300.000  5000.000
995.043    1
 8.36766550E+00 1.62199463E-02-5.52548105E-06 8.66951388E-10-
5.10674222E-14    2
 1.58330640E+04-1.82728740E+01 3.13591121E+00 1.24385956E-02
3.75791612E-05    3
-5.30731087E-08 1.97974585E-11 1.81025894E+04 1.31137225E+01
4
!C4H6-12 ATcT            C  4.H  6.   0.   0.G   200.000  6000.000 1000.
1
! 8.13872997E+00 1.68655431E-02-5.97324908E-06 9.54915173E-10-
5.67693708E-14    2
! 1.55467985E+04-1.77959041E+01 2.90828336E+00 1.79025349E-02
2.61486503E-05    3
!-4.81598832E-08 2.11295844E-11 1.75928783E+04 1.23118106E+01
1.94015186E+04    4
```

```
C4H6-13 RMG       120189C   4H   6          g  0300.00   4000.00
1000.00      1
 1.09677803E+01 1.29510755E-02-3.97761193E-06 5.74948089E-10-
3.17795241E-14    2
 8.19411540E+03-3.52875277E+01 2.73144721E+00 1.39063890E-02
4.30537876E-05    3
-6.34108493E-08 2.42036418E-11 1.14250236E+04 1.24057762E+01
4
!C4H6-13 ATcT            C  4.H  6.   0.   0.G   200.000  6000.000 1000.
1
! 7.62637466E+00 1.72523403E-02-6.09184911E-06 9.70800102E-10-
5.76169721E-14    2
! 9.55306395E+03-1.48325259E+01 4.10599669E+00 5.05575563E-03
5.83885454E-05    3
!-8.05950198E-08 3.27447711E-11 1.15092468E+04 8.42978067E+00
1.33302095E+04    4
!C4H6-13 UGhent          C   4H   6O   0     G   300.000  1500.000
1388.000     1
! 1.26945000e+01-4.20000000e-02 1.29300000e-04-1.13500000e-07
3.22800000e-11    2
! 1.06000000e+04-3.12800000e+01 1.26945000e+01-4.20000000e-02
1.29300000e-04    3
!-1.13500000e-07 3.22800000e-11 1.06000000e+04-3.12800000e+01
4
!Primary Thermo Library: Franklin (Species ID: CH2CHCHCH2)
!C4H6-13                 C   4H   6          G   300.000  5000.000
995.043    1
! 1.19566649E+01 1.22667289E-02-3.93178071E-06 5.85264319E-10-
3.30283117E-14    2
! 9.08784501E+03-4.17705168E+01 3.25557260E+00 4.77664223E-03
7.13784514E-05    3
!-9.27637286E-08 3.41969166E-11 1.29218292E+04 1.07283147E+01
4

C4H7-21 RMG             C   4H   7O   0     G   300.000  5000.000
995.043    1
 8.16992569E+00 2.06435815E-02-7.74201303E-06 1.21641928E-09-
7.05765633E-14    2
 1.24010720E+04-1.88652589E+01 3.38180293E+00 1.28954902E-02
4.46337600E-05    3
-6.11403695E-08 2.24466566E-11 1.46904000E+04 1.09264142E+01
4
!C4H7-21 ATcT            C  4.H  7.   0.   0.G   200.000  6000.000 1000.
1
! 8.08107449E+00 1.95526544E-02-6.93149115E-06 1.10889183E-09-
6.59584410E-14    2
! 1.22822959E+04-1.67137903E+01 4.54746808E+00 4.63771460E-03
6.61340221E-05    3
!-8.97456502E-08 3.61716165E-11 1.43843217E+04 7.30313471E+00
1.63702936E+04    4

!C4H7-14 RMG             C   4H   7O   0     G   300.000  5000.000
995.043    1
! 7.94091392E+00 2.03706945E-02-7.60359212E-06 1.19148613E-09-
6.90032547E-14    2
! 2.05614959E+04-1.41946431E+01 3.39149547E+00 1.24899595E-02
4.37255626E-05    3
```

```
!-5.96288908E-08 2.18523756E-11 2.27623820E+04 1.42408981E+01
4
!C4H7-14 ATcT            C  4.H  7.   0.   0.G   200.000  6000.000 1000.
1
! 8.49073768E+00 1.91056974E-02-6.74370664E-06 1.07343267E-09-
6.36251837E-14    2
! 2.04659294E+04-1.74555814E+01 5.07355313E+00 5.27619329E-03
6.23441322E-05    3
!-8.54203458E-08 3.45890031E-11 2.24615054E+04 5.60318035E+00
2.46070249E+04    4

C4H8-1 RMG              C   4H   8O   0     G   300.000  5000.000
995.043    1
 8.06996009E+00 2.30144195E-02-8.63501686E-06 1.36143870E-09-
7.92542991E-14    2
-4.35738469E+03-1.76345584E+01 3.38887348E+00 1.16753402E-02
5.39187583E-05    3
-7.10067706E-08 2.57553494E-11-1.93288526E+03 1.24275196E+01
4
!C4H8-1 ATcT             C   4H   8    0    0G   300.000  5000.    1000.
1
! 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-
0.25361045E-12    2
!-0.21397231E+04 0.15556360E+02 0.11811380E+01 0.30853380E-01
0.50865247E-05    3
!-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21075639E+02-
0.06494670E+03    4

C4H9-1 RMG              C   4H   9O   0     G   300.000  5000.000
995.043    1
 8.01071857E+00 2.56389459E-02-9.61171963E-06 1.51622055E-09-
8.83434947E-14    2
 5.10907933E+03-1.52614715E+01 3.37009523E+00 1.75812457E-02
4.28036708E-05    3
-6.05809533E-08 2.22917667E-11 7.35502735E+03 1.37488542E+01
4
!C4H9-1 ATcT             C  4.H  9.   0.   0.G   200.000  6000.000 1000.
1
! 8.97401527E+00 2.39704154E-02-8.48703645E-06 1.35644127E-09-
8.06234913E-14    2
! 5.19161526E+03-2.31075609E+01 4.73737837E+00 9.69051565E-03
6.63846383E-05    3
!-9.24799302E-08 3.74006099E-11 7.57382332E+03 4.91063455E+00
9.83838903E+03    4

nC4H10 RMG              C   4H  10O   0     G   300.000  5000.000
995.043    1
 8.14175944E+00 2.81601588E-02-1.04914204E-05 1.64919250E-09-
9.58548867E-14    2
-1.98023414E+04-1.86858146E+01 3.30538686E+00 1.69397004E-02
5.26457415E-05    3
-7.16205466E-08 2.60935571E-11-1.73219078E+04 1.22504344E+01
4
!nC4H10 ATcT             C  4.H 10.   0.   0.G   200.000  6000.000 1000.
1
! 9.44547835E+00 2.57856620E-02-9.23613194E-06 1.48631762E-09-
8.87891206E-14    2
```

```
!-2.01383773E+04-2.63477585E+01 6.14474013E+00 1.64500242E-04
9.67848789E-05    3
!-1.25486208E-07 4.97846257E-11-1.75989467E+04-1.08058878E+00-
1.51289733E+04    4

C2H4O RMG               C   2H   4O   1     G   300.000  5000.000
995.043    1
 7.49770801E+00 9.18339546E-03-3.15511448E-06 4.50622673E-10-
2.39651420E-14    2
-1.82242774E+04-1.53303849E+01 3.35283039E+00 3.95169463E-03
3.77358560E-05    3
-4.90583334E-08 1.79706017E-11-1.63155472E+04 1.00919746E+01
4
!C2H4O ATcT              C   2H   4O   1    0G   200.000  6000.000 1000.
1
! 0.68220305E+01 0.11059739E-01-0.39224574E-05 0.62778505E-09-
0.37355714E-13    2
!-0.18038769E+05-0.83716090E+01 0.30137746E+01 0.10203771E-01
0.25405637E-04    3
!-0.42341002E-07 0.18267561E-10-0.16497347E+05 0.13873511E+02-
0.14995857E+05    4

!C2H5O-1 RMG             C   2H   5O   1     G   300.000  5000.000
995.043    1
! 6.67286681E+00 1.30733710E-02-5.80233812E-06 1.01962181E-09-
6.39796503E-14    2
!-6.75820504E+03-7.61486633E+00 4.11522893E+00 3.19445102E-03
3.94811812E-05    3
!-4.96816053E-08 1.77902884E-11-5.25116047E+03 9.72667252E+00
4
C2H5O-1 ATcT            C  2.H  5.O  1.   0.G   200.000  6000.000 1000.
1
 7.02824536E+00 1.20037746E-02-4.21306455E-06 6.69471213E-10-
3.96371893E-14    2
-5.92493321E+03-9.40355948E+00 4.47893092E+00 7.59782301E-03
2.81794908E-05    3
-4.26953487E-08 1.78878934E-11-4.71446256E+03 6.38921206E+00-
2.86833500E+03    4

!C2H5O-2 RMG             C   2H   5O   1     G   300.000  5000.000
995.043    1
! 7.50435989E+00 1.20168556E-02-5.27797411E-06 9.19053674E-10-
5.73034248E-14    2
!-9.77453818E+03-1.31946344E+01 3.97920014E+00 9.45869880E-03
2.37969581E-05    3
!-3.54569452E-08 1.33270819E-11-8.24482143E+03 7.95623387E+00
4
!C2H5O-2 ATcT            C  2.H  5.O  1.   0.G   200.000  6000.000 1000.
1
! 6.35842302E+00 1.24356276E-02-4.33096839E-06 6.84530381E-10-
4.03713238E-14    2
!-9.37900432E+03-6.05106112E+00 4.22283250E+00 5.12174798E-03
3.48386522E-05    3
!-4.91943637E-08 2.01183723E-11-8.20503939E+03 8.01675700E+00-
6.49827831E+03    4
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!C3H4O RMG               C   3H   4O   1     G   300.000  5000.000
995.043    1
! 9.33734630E+00 1.14535118E-02-4.85398188E-06 8.19830986E-10-
4.99696582E-14    2
!-1.43262690E+04-2.45001170E+01 3.67436693E+00 8.66086526E-03
3.78829655E-05    3
!-5.36261068E-08 2.01146499E-11-1.19340550E+04 9.15002255E+00
4
!C3H4O ATcT              C  3.H  4.O  1.   0.G   200.000  6000.000 1000.
1
! 7.31820729E+00 1.27398510E-02-4.60112009E-06 7.44735077E-10-
4.46993049E-14    2
!-1.16137229E+04-1.11884734E+01 3.98487241E+00 3.40751550E-03
4.81227535E-05    3
!-6.61399005E-08 2.67817331E-11-9.83297241E+03 1.03960574E+01-
8.18632872E+03    4
!Primary Thermo Library: Franklin (Species ID: acrolein)
C3H4O                   C   3H   4O   1     G   300.000  5000.000
995.043    1
 8.44341329E+00 1.17202933E-02-4.18611282E-06 6.74425267E-10-
4.03914564E-14    2
-1.08501655E+04-2.01787746E+01 3.73321159E+00 9.88832349E-03
2.98806784E-05    3
-4.31239850E-08 1.62334016E-11-8.88473206E+03 7.68774200E+00
4

C3H5O-enol2 RMG         C   3H   5O   1     G   300.000  5000.000
995.043    1
 1.01157455E+01 1.24719844E-02-4.46477617E-06 6.61848794E-10-
3.64167162E-14    2
-5.17067908E+03-2.83021911E+01 3.13007173E+00 1.34496050E-02
3.49204588E-05    3
-5.31008022E-08 2.03490559E-11-2.43865897E+03 1.21074116E+01
4
!C3H5O-enol2 ATcT        C  3.H  5.O  1.   0.G   200.000  6000.000 1000.
1
! 8.15052559E+00 1.42542561E-02-5.05387276E-06 8.08732845E-10-
4.81184188E-14    2
! 8.72987262E+03-1.69520239E+01 3.53458477E+00 8.02398508E-03
4.85256807E-05    3
!-7.23549959E-08 3.03822687E-11 1.08059525E+04 1.11545728E+01
1.25165081E+04    4

C3H6O-enol2 RMG         C   3H   6O   1     G   300.000  5000.000
995.043    1
 7.08050531E+00 1.85215315E-02-7.11736789E-06 1.14075918E-09-
6.72317746E-14    2
-1.84958501E+04-9.57809052E+00 3.60782570E+00 1.30135971E-02
3.05329577E-05    3
-4.37468181E-08 1.61506364E-11-1.68409911E+04 1.20011608E+01
4
!C3H6O-enol2 ATcT        C  3.H  6.O  1.   0.G   200.000  6000.000 1000.
1
! 8.01491079E+00 1.73919953E-02-6.26027968E-06 1.01188256E-09-
6.06239111E-14    2
!-1.51980838E+04-1.88279964E+01 3.42806676E+00 6.25176642E-03
6.13196311E-05    3
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!-8.60387185E-08 3.51371393E-11-1.28446646E+04 1.04244994E+01-
1.11564001E+04    4

!C3H7O-N1 RMG            C   3H   7O   1     G   300.000  5000.000
995.043    1
! 8.80032645E+00 1.91143969E-02-8.13211711E-06 1.39545792E-09-
8.62604933E-14    2
!-1.03103341E+04-1.71908542E+01 3.92707025E+00 1.37424883E-02
3.75954967E-05    3
!-5.44528754E-08 2.02796269E-11-8.10475568E+03 1.25051479E+01
4
!Primary Thermo Library: Burcat (Species ID: C3H7O-N1)
C3H7O-N1                C   3H   7O   1     G   300.000  5000.000
995.043    1
 8.05956830E+00 1.84740293E-02-6.63766463E-06 1.07861962E-09-
6.50761319E-14    2
-1.13500046E+04-1.21440907E+01 3.85193622E+00 1.23321505E-02
3.73777310E-05    3
-5.16977214E-08 1.90453830E-11-9.37123823E+03 1.38698819E+01
4

C3H7O-N2 RMG            C   3H   7O   1     G   300.000  5000.000
995.043    1
 7.49949916E+00 2.08102131E-02-9.06038673E-06 1.58200187E-09-
9.89891093E-14    2
-1.12292755E+04-9.40563157E+00 4.20675393E+00 1.16221333E-02
3.85949874E-05    3
-5.29951943E-08 1.93036606E-11-9.46384603E+03 1.20419757E+01
4

C3H7O-N3 RMG            C   3H   7O   1     G   300.000  5000.000
995.043    1
 9.57276776E+00 1.82190254E-02-7.72954286E-06 1.32180309E-09-
8.14995710E-14    2
-1.33121421E+04-2.24692288E+01 3.83103341E+00 1.97596519E-02
2.24200714E-05    3
-4.06339684E-08 1.59257682E-11-1.11031031E+04 1.05612736E+01
4

C4H9O-1 RMG             C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.07502372E+01 2.54790904E-02-1.06157981E-05 1.80002028E-09-
1.10422093E-13    2
-1.38539276E+04-2.57496673E+01 3.77054036E+00 2.42311317E-02
3.54432176E-05    3
-5.86575262E-08 2.25157679E-11-1.10141080E+04 1.51787892E+01
4

C4H9O-2 RMG             C   4H   9O   1     G   300.000  5000.000
995.043    1
 8.23855797E+00 2.85144390E-02-1.18023623E-05 2.00078861E-09-
1.22852800E-13    2
-1.42562078E+04-1.07703272E+01 4.00331953E+00 2.34902912E-02
2.90104275E-05    3
-4.76130335E-08 1.79375685E-11-1.23217874E+04 1.51262518E+01
4
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C4H9O-3 RMG             C   4H   9O   1     G   300.000  5000.000
995.043    1
 9.60366290E+00 2.68532519E-02-1.13750461E-05 1.95358081E-09-
1.20939420E-13    2
-1.47710363E+04-1.88416772E+01 4.01144448E+00 2.22255059E-02
3.64658202E-05    3
-5.74780557E-08 2.16897986E-11-1.23161388E+04 1.48531730E+01
4

C4H9O-4 RMG             C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.15947540E+01 2.44705227E-02-1.01512701E-05 1.71398112E-09-
1.04819295E-13    2
-1.68795457E+04-3.14239392E+01 3.65742738E+00 3.03468822E-02
2.02314839E-05    3
-4.49332331E-08 1.82206113E-11-1.40112660E+04 1.33051478E+01
4

C4H9O-5 RMG             C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.09424660E+01 2.58890155E-02-1.07647566E-05 1.82339572E-09-
1.11774144E-13    2
-1.25209072E+04-2.96622400E+01 3.75053043E+00 2.18564872E-02
4.49757373E-05    3
-6.87947146E-08 2.59903101E-11-9.45876145E+03 1.31940211E+01
4
!C4H9O-5 ATcT            C  4.H  9.O  1.   0.G   200.000  6000.000 1000.
1
! 1.21336180E+01 2.43954328E-02-9.04409323E-06 1.48350965E-09-
8.96467065E-14    2
!-1.29883091E+04-3.89685328E+01 5.61984431E+00 2.12772932E-03
1.02679749E-04    3
!-1.34097807E-07 5.25493048E-11-9.21442557E+03 4.46683857E+00-
6.77732206E+03    4

nC4H10O RMG             C   4H  10O   1     G   300.000  5000.000
995.043    1
 1.08812781E+01 2.80003033E-02-1.14954988E-05 1.93299223E-09-
1.17933485E-13    2
-3.87653483E+04-2.92243325E+01 3.70583199E+00 2.35895864E-02
4.52852882E-05    3
-6.96971195E-08 2.63175583E-11-3.56910432E+04 1.36300474E+01
4
!nC4H10O ATcT            C   4H  10O   1    0G   200.000  6000.000 1000.
1
! 0.13084060E+02 0.26489386E-01-0.10030766E-04 0.16703993E-08-
0.10204842E-12    2
!-0.39853115E+05-0.42581058E+02 0.59455772E+01 0.23216158E-02
0.10865741E-03    3
!-0.14026051E-06 0.54446937E-10-0.35620542E+05 0.52265747E+01-
0.33036174E+05    4

nC4H8O                  C   4H   8O   1     G   300.000  5000.000
995.043    1
 9.57363195E+00 2.46958431E-02-1.01184795E-05 1.69848620E-09-
1.03515441E-13    2
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-2.95034981E+04-2.19876450E+01 3.76176479E+00 2.57747745E-02
2.18481205E-05    3
-4.22256955E-08 1.65870049E-11-2.72436886E+04 1.15658436E+01
4
C3H5O-nal               C   3H   5O   1     G   300.000  5000.000
995.043    1
 7.30437846E+00 1.61279912E-02-6.90069394E-06 1.18770816E-09-
7.35820846E-14    2
-1.02016110E+03-8.88716459E+00 4.01299949E+00 1.64406437E-02
1.21022083E-05    3
-2.45914981E-08 9.68145008E-12 2.74386024E+02 1.01890830E+01
4
C4H7O                   C   4H   7O   1     G   300.000  5000.000
995.043    1
 9.88387426E+00 2.15106253E-02-8.09054069E-06 1.27247621E-09-
7.38733718E-14    2
-7.95217089E+03-2.41962679E+01 3.25015824E+00 2.12430218E-02
3.29161372E-05    3
-5.34052070E-08 2.04984549E-11-5.29859055E+03 1.44748959E+01
4
C3H6O-nal               C   3H   6O   1     G   300.000  5000.000
995.043    1
 7.49791166E+00 1.86108376E-02-7.81858837E-06 1.33296944E-09-
8.20849841E-14    2
-2.59701067E+04-1.27049209E+01 3.97369033E+00 1.51206037E-02
2.40608191E-05    3
-3.78595713E-08 1.42455058E-11-2.43946205E+04 8.67235040E+00
4
C4H6O                   C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.05999067E+01 1.85214656E-02-7.64851316E-06 1.28159650E-09-
7.78688192E-14    2
-1.90601631E+04-2.95735976E+01 3.60617265E+00 1.92822501E-02
3.24393153E-05    3
-5.32035109E-08 2.05523631E-11-1.63142003E+04 1.09368516E+01
4
C4H8O-enol              C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.12861336E+01 2.18491858E-02-8.05365585E-06 1.24364286E-09-
7.11119413E-14    2
-2.66322315E+04-3.22078119E+01 3.02258658E+00 2.25385344E-02
3.99445278E-05    3
-6.37690004E-08 2.45175500E-11-2.33773250E+04 1.57100236E+01
4
C4H8-2                  C   4H   8O   0     G   300.000  5000.000
995.043    1
 6.81444858E+00 2.44229463E-02-9.22688262E-06 1.46695868E-09-
8.60241491E-14    2
-5.38642039E+03-1.09669333E+01 3.53636731E+00 1.40189647E-02
4.20055070E-05    3
-5.66753048E-08 2.05059156E-11-3.56663357E+03 1.06978063E+01
4
C4H9-2                  C   4H   9O   0     G   300.000  5000.000
995.043    1
 5.49903935E+00 2.86742945E-02-1.07982839E-05 1.71698889E-09-
1.00774201E-13    2
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 4.70679917E+03-2.82131411E-01 3.60287439E+00 1.68404053E-02
3.63708807E-05    3
-4.95364606E-08 1.77135673E-11 6.04734795E+03 1.36963168E+01
4
C4H8O-enol3             C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.09703254E+01 2.24914624E-02-9.39987269E-06 1.59436443E-09-
9.77719559E-14    2
-2.33716732E+04-2.89944344E+01 3.71700136E+00 1.83395158E-02
4.70726716E-05    3
-6.98840644E-08 2.63133874E-11-2.02791819E+04 1.42487809E+01
4
C4H5-4                  C   4H   5O   0     G   300.000  5000.000
995.043    1
 6.99580278E+00 1.61744073E-02-5.60544638E-06 8.20832653E-10-
4.49110687E-14    2
 4.13033611E+04-8.82099524E+00 3.23920339E+00 1.79518417E-02
1.18004221E-05    3
-2.42978000E-08 9.64701981E-12 4.27105591E+04 1.25982003E+01
4

!C4H6-1                  C   4H   6O   0     G   300.000  5000.000
995.043    1
! 7.11381994E+00 1.86476725E-02-6.42531114E-06 9.39275620E-10-
5.13490337E-14    2
! 1.64515474E+04-1.21508345E+01 3.15157920E+00 1.74587936E-02
2.11700034E-05    3
!-3.48370264E-08 1.32807602E-11 1.80874430E+04 1.12029832E+01
4
C4H6-1 ATcT             C   4H   6O   0     G   200.000  6000.000
1000.000    1
 7.81179394E+00 1.79733772E-02-6.61044149E-06 1.05501491E-09-
6.19297169E-14    2
 1.61770171E+04-1.59658015E+01 2.42819263E+00 2.49821955E-02
6.27370548E-06    3
-2.61747866E-08 1.26585079E-11 1.80248564E+04 1.36683982E+01
4

C4H7-12                 C   4H   7O   0     G   300.000  5000.000
995.043    1
 7.51589729E+00 2.08850669E-02-7.83356591E-06 1.23395938E-09-
7.17899904E-14    2
 2.47677939E+04-1.24319038E+01 3.45288308E+00 1.52014012E-02
3.39239676E-05    3
-4.89796909E-08 1.81310094E-11 2.66663158E+04 1.26264866E+01
4

!C4H7-11                 C   4H   7O   0     G   300.000  5000.000
995.043    1
! 8.42885739E+00 1.98226731E-02-7.37321686E-06 1.15073056E-09-
6.64153001E-14    2
! 2.55215037E+04-1.78308710E+01 3.33891290E+00 1.48283185E-02
3.85292086E-05    3
!-5.53131714E-08 2.05793635E-11 2.77946367E+04 1.30322178E+01
4
C4H7-11 ATcT            C   4H   7O   0     G   200.000  6000.000
1000.000    1
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 8.15650000E+00 1.90310000E-02-6.73260000E-06 1.07330000E-09-
6.36890000E-14    2
 2.55826427E+04-1.61429000E+01 4.19860000E+00 1.19620000E-02
4.23860000E-05    3
-6.30300000E-08 2.59480000E-11 2.75256555E+04 8.57180000E+00
4

C4H6O-enol              C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.31128438E+01 1.41689598E-02-4.84646545E-06 6.87826014E-10-
3.63485551E-14    2
-1.38298392E+04-4.35303204E+01 2.71845138E+00 2.22906331E-02
3.36564410E-05    3
-5.91079383E-08 2.35292326E-11-1.00947607E+04 1.49389986E+01
4
C4H7O-13                C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.07042999E+01 2.06018470E-02-8.71846682E-06 1.48716285E-09-
9.14923712E-14    2
-6.37266285E+03-2.89306955E+01 3.75030540E+00 1.44302776E-02
5.20292133E-05    3
-7.36800489E-08 2.74536073E-11-3.29932740E+03 1.30729881E+01
4
C4H7O-23                C   4H   7O   1     G   300.000  5000.000
995.043    1
 7.73362963E+00 2.36127629E-02-9.25772260E-06 1.50957745E-09-
9.01886880E-14    2
 5.91166845E+03-9.14819176E+00 3.66140560E+00 2.71075602E-02
4.88305331E-06    3
-2.09684271E-08 8.82446815E-12 7.35947157E+03 1.36805539E+01
4
C4H8O-enol2             C   4H   8O   1     G   300.000  5000.000
995.043    1
 8.41562201E+00 2.55318629E-02-9.90296761E-06 1.60238216E-09-
9.51730755E-14    2
-2.32722582E+04-1.51021795E+01 3.53995267E+00 2.30680458E-02
2.70715317E-05    3
-4.54541282E-08 1.73263271E-11-2.12096859E+04 1.38844470E+01
4

C2H3O-1 rmg             C   2H   3O   1     G   300.000  5000.000
995.043    1
 7.68500561E+00 6.34913743E-03-2.12423131E-06 2.88818555E-10-
1.45459633E-14    2
 1.17256799E+04-1.45548679E+01 3.37355471E+00 7.66274450E-03
2.00424136E-05    3
-3.07406795E-08 1.18461530E-11 1.33766804E+04 1.02086415E+01
4
C2H3O-2 rmg             C   2H   3O   1     G   300.000  5000.000
995.043    1
 7.68500561E+00 6.34913743E-03-2.12423131E-06 2.88818555E-10-
1.45459633E-14    2
 1.17256799E+04-1.45548679E+01 3.37355471E+00 7.66274450E-03
2.00424136E-05    3
-3.07406795E-08 1.18461530E-11 1.33766804E+04 1.02086415E+01
4
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C3H5O-21 rmg            C   3H   5O   1     G   300.000  5000.000
995.043    1
 1.01157455E+01 1.24719844E-02-4.46477617E-06 6.61848794E-10-
3.64167172E-14    2
-5.17067908E+03-2.83021911E+01 3.13007173E+00 1.34496050E-02
3.49204588E-05    3
-5.31008022E-08 2.03490559E-11-2.43865897E+03 1.21074116E+01
4
C3H5O-24 rmg            C   3H   5O   1     G   300.000  5000.000
995.043    1
 7.25054101E+00 1.62457723E-02-6.23020280E-06 9.94544085E-10-
5.84042668E-14    2
-4.21529774E+03-1.18369384E+01 3.58884681E+00 1.31436859E-02
2.53120373E-05    3
-3.81382250E-08 1.42959077E-11-2.60431043E+03 1.02437939E+01
4
C3H5O-31 rmg            C   3H   5O   1     G   300.000  5000.000
995.043    1
 7.30437846E+00 1.61279912E-02-6.90069394E-06 1.18770816E-09-
7.35820846E-14    2
-1.02016110E+03-8.88716459E+00 4.01299949E+00 1.64406437E-02
1.21022083E-05    3
-2.45914981E-08 9.68145008E-12 2.74386024E+02 1.01890830E+01
4
C4H6O-13 rmg            C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.31128438E+01 1.41689598E-02-4.84646545E-06 6.87826014E-10-
3.63485551E-14    2
-1.37795172E+04-4.35303204E+01 2.71845138E+00 2.22906331E-02
3.36564410E-05    3
-5.91079383E-08 2.35292326E-11-1.00444387E+04 1.49389986E+01
4
C4H6O-24 rmg            C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.05999067E+01 1.85214656E-02-7.64851316E-06 1.28159650E-09-
7.78688192E-14    2
-1.90601631E+04-2.95735976E+01 3.60617265E+00 1.92822501E-02
3.24393153E-05    3
-5.32035109E-08 2.05523631E-11-1.63142003E+04 1.09368516E+01
4
C4H7O-13 rmg            C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.07042999E+01 2.06018470E-02-8.71846682E-06 1.48716285E-09-
9.14923712E-14    2
-6.37266285E+03-2.89306955E+01 3.75030540E+00 1.44302776E-02
5.20292133E-05    3
-7.36800489E-08 2.74536073E-11-3.29932740E+03 1.30729881E+01
4
!C4H7O-14 rmg            C   4H   7O   1     G   300.000  5000.000
995.043    1
! 1.15249493E+01 1.92022713E-02-8.14314256E-06 1.38924670E-09-
8.54790549E-14    2
!-1.43719357E+03-3.03571108E+01 3.67882763E+00 2.52555959E-02
2.11533756E-05    3
!-4.39811706E-08 1.77812203E-11 1.38602422E+03 1.37971918E+01
4
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C4H7O-32 rmg            C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.10123148E+01 2.00211608E-02-7.47090541E-06 1.16143215E-09-
6.67140293E-14    2
-9.63382628E+03-3.20309102E+01 3.10225204E+00 1.89416017E-02
4.37183487E-05    3
-6.63405918E-08 2.52356817E-11-6.43204183E+03 1.42698753E+01
4
C4H7O-35 rmg            C   4H   7O   1     G   300.000  5000.000
995.043    1
 9.88387426E+00 2.15106253E-02-8.09054069E-06 1.27247621E-09-
7.38733718E-14    2
-7.95217089E+03-2.41962679E+01 3.25015824E+00 2.12430218E-02
3.29161372E-05    3
-5.34052070E-08 2.04984549E-11-5.29859055E+03 1.44748959E+01
4
C4H7-24 rmg             C   4H   7O   0     G   300.000  5000.000
995.043    1
 8.16992569E+00 2.06435815E-02-7.74201303E-06 1.21641928E-09-
7.05765633E-14    2
 1.24010720E+04-1.88652589E+01 3.38180293E+00 1.28954902E-02
4.46337600E-05    3
-6.11403695E-08 2.24466566E-11 1.46904000E+04 1.09264142E+01
4

!C4H5-113 RMG            C   4H   5O   0     G   300.000  5000.000
995.043    1
! 6.49266056E+00 1.68368773E-02-5.45924754E-06 7.50059603E-10-
3.86696159E-14    2
! 3.43960771E+04-7.96071084E+00 3.03787313E+00 1.96385363E-02
7.02967924E-06    3
!-1.88144450E-08 7.69003801E-12 3.56324440E+04 1.14473175E+01
4
C4H5-113 ATcT           C   4H   5O   0     G   200.000  6000.000
1000.000    1
 9.21468577E+00 1.34950214E-02-4.82557552E-06 7.76743641E-10-
4.64080569E-14    2
 3.40842790E+04-2.25150877E+01 2.15910182E+00 3.04425273E-02-
1.62521254E-05    3
-1.73750743E-10 2.43871422E-12 3.62155591E+04 1.46844795E+01
4

!nC4H5 RMG               C   4H   5O   0     G   300.000  5000.000
995.043    1
! 1.04306375E+01 1.18071498E-02-3.95818547E-06 5.51468424E-10-
2.86323786E-14    2
! 3.83019523E+04-3.01376345E+01 2.97255253E+00 1.42343438E-02
3.39194437E-05    3
!-5.26550800E-08 2.03311812E-11 4.11502383E+04 1.26605457E+01
4
nC4H5 ATcT              C   4H   5O   0     G   200.000  6000.000
1000.000    1
 8.11183574E+00 1.42276370E-02-5.02419535E-06 8.00816580E-10-
4.75459802E-14    2
 4.00134524E+04-1.52704514E+01 3.28605952E+00 1.43352325E-02
2.78456642E-05    3
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-4.84612551E-08 2.10628469E-11 4.19222504E+04 1.26653969E+01
4

!iC4H5    RMG            C   4H   5O   0     G   300.000  5000.000
995.043    1
! 8.94642571E+00 1.46679861E-02-5.42142561E-06 8.34035913E-10-
4.74778835E-14    2
! 3.35990859E+04-2.27620527E+01 3.30543668E+00 1.32896428E-02
3.29182143E-05    3
!-4.91480461E-08 1.86142996E-11 3.59125316E+04 1.04082920E+01
4
iC4H5 ATcT              C   4H   5O   0     G   200.000  6000.000
1000.000    1
 8.58761100E+00 1.42683804E-02-5.04812095E-06 8.06555355E-10-
4.79335634E-14    2
 3.40836919E+04-1.96196761E+01 2.00881066E+00 2.50340684E-02
4.47930427E-06    3
-2.63989791E-08 1.34432880E-11 3.62069792E+04 1.59913722E+01
4
!Primary Thermo Library: Franklin (Species ID: CH2CHCCH2)
!iC4H5                  C   4H   5          G   300.000  5000.000
995.043    1
! 9.10109944E+00 1.34516723E-02-4.57980040E-06 7.12492366E-10-
4.16245209E-14    2
! 3.93833754E+04-7.53014693E+00 3.57286186E+00 1.30717177E-02
3.00664857E-05    3
!-4.53289459E-08 1.72617226E-11 4.16025184E+04 2.47356863E+01
4

C3H6O-enol rmg          C   3H   6O   1     G   300.000  5000.000
995.043    1
 8.70653438E+00 1.64178410E-02-6.07148186E-06 9.39049461E-10-
5.37535696E-14    2
-2.29418616E+04-2.01261739E+01 3.32295563E+00 1.45061390E-02
3.23163168E-05    3
-4.85688780E-08 1.83616588E-11-2.07044653E+04 1.16788626E+01
4

C6H9J(100)              C   6H   90   00   0G   300.000  5000.000
1394.000     1
 1.69487032E+01 2.02481619E-02-6.64585754E-06 1.00419717E-09-
5.72732423E-14    2
 1.87327194E+04-6.29267286E+01-2.17789081E+00 6.81151267E-02-
5.30992660E-05    3
 2.17165926E-08-3.61564699E-12 2.50250938E+04 3.86137921E+01
4
C6H9J(191)              C   6H   90   00   0G   300.000  5000.000
1375.000     1
 1.39945981E+01 2.47091437E-02-8.41731699E-06 1.30270056E-09-
7.54500419E-14    2
 1.47015860E+04-5.22656061E+01-3.55701930E+00 5.82957778E-02-
2.94970992E-05    3
 5.42890366E-09 6.37120883E-14 2.15275615E+04 4.46115467E+01
4
C6H8(248)               C   6H   80   00   0G   300.000  5000.000
1391.000     1
```

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 1.52456723E+01 2.05599099E-02-6.84210627E-06 1.04457084E-09-
6.00124896E-14    2
 5.15799212E+03-5.92776844E+01-5.34580312E+00 6.95506709E-02-
5.12381271E-05    3
 1.92721048E-08-2.92115911E-12 1.21545557E+04 5.08884254E+01
4
C6H7J(266)              C   6H   70   00   0G   300.000  5000.000
1397.000     1
 1.54016860E+01 1.76385824E-02-5.76677925E-06 8.70770395E-10-
4.96881023E-14    2
 1.69101171E+04-6.16012943E+01-5.49292445E+00 7.14235834E-02-
5.92049381E-05    3
 2.50978969E-08-4.25198580E-12 2.35838359E+04 4.87105548E+01
4
C6H10(96)               C   6H  100   00   0G   300.000  5000.000
1389.000     1
 1.71030051E+01 2.22520476E-02-7.36290668E-06 1.12019727E-09-
6.41933515E-14    2
 1.61094466E+03-6.40863020E+01-1.58111740E+00 6.60376180E-02-
4.66425841E-05    3
 1.72030216E-08-2.60295960E-12 8.07157628E+03 3.61878490E+01
4
C3H6O                   C   3H   6O   10   0G   300.000  5000.000
2018.000     1
 1.06712054E+01 1.34039627E-02-5.04777716E-06 8.42754566E-10-
5.14368781E-14    2
-2.73990500E+04-3.07467312E+01 2.07996455E+00 2.96842348E-02-
1.44301489E-05    3
 2.13725578E-09 1.48023247E-13-2.42118877E+04 1.65088661E+01
4
C3H5OJ(8)               C   3H   5O   10   0G   300.000  5000.000
1685.000     1
 1.03844973E+01 1.11780244E-02-4.32036702E-06 7.32673613E-10-
4.51362326E-14    2
-8.52074616E+03-2.76582578E+01 2.86275348E+00 2.48426510E-02-
1.13352498E-05    3
 1.07715766E-09 2.97933397E-13-5.68469243E+03 1.39174782E+01
4
C3H5OJ(12)              C   3H   5O   10   0G   300.000  5000.000
1572.000     1
 1.17474332E+01 9.26150465E-03-3.58839644E-06 6.07197991E-10-
3.72176989E-14    2
-4.80471605E+03-3.44275120E+01 3.97527027E+00 1.66990940E-02
2.57202140E-06    3
-8.25590374E-09 2.46621228E-12-1.02913335E+03 1.11276401E+01
4
C3H5OJ(13)              C   3H   5O   10   0G   300.000  5000.000
2012.000     1
 1.03853667E+01 1.11388812E-02-4.28565147E-06 7.24993728E-10-
4.46001937E-14    2
-2.47481488E+03-2.64675847E+01 2.88397505E+00 2.49687038E-02-
1.16950722E-05    3
 1.34153197E-09 2.39050282E-13 3.45317252E+02 1.49302812E+01
4
C4H7OJ(8)               C   4H   7O   10   0G   300.000  5000.000
1364.000     1
```

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 1.52900714E+01 1.33896524E-02-4.84842512E-06 7.86686991E-10-
4.70230432E-14    2
-1.35873616E+04-5.35024043E+01 3.05234023E+00 3.47293957E-02-
1.52769867E-05    3
 7.61891817E-10 7.02868701E-13-8.61142482E+03 1.47974889E+01
4
C2H3OJ(10)              C   2H   3O   10   0G   300.000  5000.000
1370.000     1
 7.05095008E+00 6.91334555E-03-2.35358993E-06 3.64944162E-10-
2.11689491E-14    2
-1.72653486E+02-1.15088831E+01 2.96334537E+00 1.38410015E-02-
5.49232775E-06    3
 1.60818335E-10 2.66299170E-13 1.51867102E+03 1.13905617E+01
4
C4H7OJ(12)              C   4H   7O   10   0G   300.000  5000.000
1681.000     1
 1.26854321E+01 1.66344856E-02-6.42017234E-06 1.08565102E-09-
6.67286697E-14    2
-7.53930203E+03-3.68208701E+01 3.11300817E+00 3.23671408E-02-
1.20232490E-05    3
-6.30291504E-10 8.23640788E-13-3.76949333E+03 1.66843717E+01
4
C4H7OJ(13)              C   4H   7O   10   0G   300.000  5000.000
1682.000     1
 1.12090089E+01 1.84045154E-02-6.89653012E-06 1.14207401E-09-
6.92539913E-14    2
-6.95560096E+03-2.80687989E+01 3.96746306E+00 2.79613867E-02-
6.47489016E-06    3
-3.14934613E-09 1.22945888E-12-3.87265970E+03 1.32567444E+01
4
C4H7OJ(16)              C   4H   7O   10   0G   300.000  5000.000
1365.000     1
 1.52574660E+01 1.33941462E-02-4.83288501E-06 7.82499234E-10-
4.67126485E-14    2
-7.46229052E+03-5.21096978E+01 3.05986324E+00 3.49345775E-02-
1.57986181E-05    3
 1.15659430E-09 6.08679615E-13-2.52933213E+03 1.58708587E+01
4
C4H7-22                 C   4H   7          G   300.000  5000.000
995.043    1
 7.25106656E+00 2.01441616E-02-7.20543150E-06 1.17172485E-09-
7.08224242E-14    2
 2.34929821E+04-1.08979675E+01 3.41175053E+00 2.04834535E-02
1.50376158E-05    3
-2.89761032E-08 1.13339844E-11 2.50042987E+04 1.13603469E+01
4
C4H6-2                  C   4H   6          G   300.000  5000.000
995.043    1
 6.11833579E+00 1.89033993E-02-5.80539604E-06 8.27720234E-10-
4.51607937E-14    2
 1.43697219E+04-7.25608073E+00 2.87966261E+00 1.78421808E-02
1.70202591E-05    3
-2.86862888E-08 1.09430864E-11 1.57113054E+04 1.18552131E+01
4

C4H7OJ(39)              C   4H   7O   1     G   300.000  5000.000
995.043    1
```

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 1.05271730E+01 1.97023672E-02-7.74611024E-06 1.34444366E-09-
8.47994459E-14    2
-1.09694167E+04-2.53119922E+01 3.61454504E+00 2.90201570E-02
6.05131381E-06    3
-2.65546340E-08 1.16116945E-11-8.67935436E+03 1.25978173E+01
4
C3H7O2                  C   3H   7O   2     G   300.000  5000.000
995.043    1
 1.09424455E+01 1.89567444E-02-7.35344246E-06 1.26726334E-09-
7.95918067E-14    2
-9.30087603E+03-2.73164451E+01 3.51459651E+00 2.72103115E-02
1.27747596E-05    3
-3.40400513E-08 1.42738053E-11-6.75306207E+03 1.38564051E+01
4
CH2CH2CH2OOH            C   3H   7O   2     G   300.000  5000.000
995.043    1
 1.27660544E+01 1.74576686E-02-7.03981612E-06 1.24261252E-09-
7.91833233E-14    2
-3.43467768E+03-3.60130774E+01 3.50571681E+00 2.98664314E-02
1.16654531E-05    3
-3.63547069E-08 1.56644448E-11-3.63206935E+02 1.47902041E+01
4
aC3H5O2                 C   3H   5O   2     G   300.000  5000.000
995.043    1
 8.92185497E+00 1.62632359E-02-5.74054085E-06 9.24531735E-10-
5.55133414E-14    2
 7.47691436E+03-1.53907755E+01 3.21714447E+00 2.71581466E-02-
4.01794829E-06    3
-1.23874370E-08 6.34366411E-12 9.20812868E+03 1.50972901E+01
4
nSPC(301)               C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.61719097E+01 2.35746991E-02-8.84799580E-06 1.49673961E-09-
9.29610923E-14    2
-3.41165397E+04-5.02201811E+01 3.13615544E+00 4.74714742E-02-
1.89969286E-06    3
-3.19492906E-08 1.55437489E-11-3.01111084E+04 1.96961920E+01
4
nSPC(351)               C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.87965704E+01 2.11602406E-02-8.13425521E-06 1.39997052E-09-
8.79317260E-14    2
-3.12651586E+04-6.43509697E+01 3.03483515E+00 5.62437769E-02-
1.83941711E-05    3
-2.02859632E-08 1.25361204E-11-2.67285465E+04 1.86462935E+01
4
nSPC(385)               C   4H   8O   3     G   300.000  5000.000
995.043    1
 1.66196012E+01 2.17457871E-02-8.31898109E-06 1.42064712E-09-
8.87178023E-14    2
-4.38776565E+04-5.40569565E+01 3.12525790E+00 5.16363105E-02-
1.66624860E-05    3
-1.75883470E-08 1.08676041E-11-3.99864224E+04 1.70371445E+01
4
nSPC(447)               C   4H   7O   2     G   300.000  5000.000
995.043    1
```

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 1.35727516E+01 1.92920497E-02-7.45894898E-06 1.28257624E-09-
8.04358489E-14    2
-2.47462377E+04-4.00958708E+01 3.32349143E+00 3.67973522E-02
1.87333259E-06    3
-2.89026131E-08 1.35164325E-11-2.15334656E+04 1.51945798E+01
4
!Primary Thermo Library: Lee&Bozzelli_JPCA_107_19_3778 (Species ID:
nSPC(543))
nSPC(543)              C   2H   3O   3     G   250.000  5000.000
995.043    1
 1.19720189E+01 6.95582270E-03-1.65824164E-06 1.70655329E-10-
6.11045705E-15    2
-1.56466583E+04-3.28049146E+01 2.98164243E+00 8.41511954E-03
4.84231271E-05    3
-6.84110447E-08 2.60253047E-11-1.21405778E+04 1.91511376E+01
4
nSPC(801)              C   2H   3O   3     G   300.000  5000.000
995.043    1
 1.19358756E+01 7.85869745E-03-2.93713453E-06 4.96883404E-10-
3.08572494E-14    2
-2.26291362E+04-3.25166203E+01 3.08441548E+00 2.49455753E-02-
8.13898358E-07    3
-1.96057547E-08 9.71312923E-12-1.99519981E+04 1.47434870E+01
4
nSPC(879)              C   2H   3O   5     G   300.000  5000.000
995.043    1
 1.79003120E+01 5.78663645E-03-1.33539951E-06 1.42820031E-10-
5.62968880E-15    2
-4.00278289E+04-6.00060980E+01 2.19206476E+00 3.23704588E-02
1.37067275E-05    3
-4.68626265E-08 2.10821193E-11-3.50917233E+04 2.47942890E+01
4
nSPC(1064)             C   2H   2O   4     G   300.000  5000.000
995.043    1
 1.39157467E+01 4.64550330E-03-1.54986926E-06 2.49508614E-10-
1.50363591E-14    2
-2.17725218E+04-4.22133535E+01 2.81906698E+00 1.62403754E-02
3.07373444E-05    3
-5.47252685E-08 2.21743389E-11-1.79298634E+04 1.94788976E+01
4
nSPC(102)              C   1H   2O   2     G   300.000  5000.000
995.043    1
 5.24521848E+00 7.08443192E-03-2.43091075E-06 3.82228849E-10-
2.25633707E-14    2
 2.37759113E+04 1.53855051E-01 3.37295085E+00 1.37363923E-02-
1.11403961E-05    3
 5.33432475E-09-1.04486655E-12 2.41917971E+04 9.39468109E+00
4

!KVG, UGhent
C6H10                  C   6H  10          G   300.000  5000.000
995.043    1
 1.29787965E+01 2.87323534E-02-1.00125826E-05 1.58807804E-09-
9.40765408E-14    2
-7.56868863E+03-4.86741107E+01 2.82778418E+00 6.58222237E-03
1.18283305E-04    3
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-1.47953937E-07 5.34532022E-11-2.43185857E+03 1.59093044E+01
4
C8H8 Styrene      P 4/89C  8.H  8.   0.   0.G   200.000  6000.000 1000.
1
 1.39192973E+01 2.94553961E-02-1.02697803E-05 1.31095793E-09-
6.16742309E-14    2
 1.09344570E+04-4.97233295E+01 1.18176309E+00 3.34877555E-02
6.92369418E-05    3
-1.24490988E-07 5.49387246E-11 1.56039775E+04 2.26626016E+01
1.78362886E+04    4
C8H9 C6H5CH2CH2*  A11/04C  8.H  9.   0.   0.G   200.000  6000.000 1000.
1
 1.61326962E+01 2.82904273E-02-1.01801876E-05 1.64176637E-09-
9.81375329E-14    2
 2.08791061E+04-6.00115413E+01 7.33299107E-01 4.59053158E-02
3.78257231E-05    3
-9.12367411E-08 4.25589678E-11 2.61572945E+04 2.50411074E+01
2.85902549E+04    4
C7H8  Toluene     g 1/93C  7.H  8.   0.   0.G   200.000  6000.000 1000.
1
 1.29393610E+01 2.66922277E-02-9.68422041E-06 1.57392386E-09-
9.46671699E-14    2
-6.76971149E+02-4.67249759E+01 1.61200102E+00 2.11179855E-02
8.53239986E-05    3
-1.32568501E-07 5.59411406E-11 4.09654820E+03 2.02969771E+01
6.03402967E+03    4
C7H9                    C   7H   90   00   0G   300.000  5000.000
1392.000     1
 1.72345420E+01 2.48843728E-02-8.27015777E-06 1.25495450E-09-
7.17094105E-14    2
 1.26511384E+04-7.07657879E+01-5.49639130E+00 7.99171938E-02-
5.94935991E-05    3
 2.30449422E-08-3.63904531E-12 2.03047656E+04 5.05507938E+01
4
C6H9_1_2_5              C   6H   90   00   0G   300.000  5000.000
1394.000     1
 1.69217162E+01 2.02745051E-02-6.64939177E-06 1.00413073E-09-
5.72454107E-14    2
 1.87471882E+04-6.27655758E+01-2.18694516E+00 6.81744607E-02-
5.32242977E-05    3
 2.18126748E-08-3.63901712E-12 2.50260820E+04 3.86524442E+01
4
C6H9_CYC_1_3            C   6H   90   00   0G   300.000  5000.000
1375.000     1
 1.39824255E+01 2.47190719E-02-8.41817157E-06 1.30255577E-09-
7.54309194E-14    2
 1.47083903E+04-5.21919564E+01-3.55973355E+00 5.83175535E-02-
2.95502555E-05    3
 5.47121817E-09 5.32998409E-14 2.15277938E+04 4.46225284E+01
4
C6H8_CYC_1_4            C   6H   80   00   0G   300.000  5000.000
1391.000     1
 1.52456723E+01 2.05599099E-02-6.84210627E-06 1.04457084E-09-
6.00124896E-14    2
 5.15799212E+03-5.92776844E+01-5.34580312E+00 6.95506709E-02-
5.12381271E-05    3
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 1.92721048E-08-2.92115911E-12 1.21545557E+04 5.08884254E+01
4
!Burcat 30-SEPT-2010
C6H7_CYC_1_2  Ene T 8/10C  6.H  7.   0.   0.G   200.000  6000.000 1000.
1
 1.14416904E+01 2.28023386E-02-8.21084119E-06 1.32793102E-09-
7.96046682E-14    2
 1.95096674E+04-3.89180376E+01 9.89769161E-01 2.08229745E-02
7.09544962E-05    3
-1.14720397E-07 4.92346711E-11 2.37120517E+04 2.20321792E+01
2.53560814E+04    4
C6H10_CYC               C   6H  10O   0     G   300.000  1500.000
1
-4.81125000e-01 5.98700000e-02-3.59000000e-05 8.94200000e-09-
2.85100000e-13    2
 8.17300000e+03 3.22200000e+01-4.81125000e-01 5.98700000e-02-
3.59000000e-05    3
 8.94200000e-09-2.85100000e-13 8.17300000e+03 3.22200000e+01
4

! The following NASA-7 polynomials are from study by:
!    Sharma, S. "Modeling of 1,3-hexadiene, 2,4-hexadiene, and 1,4-
hexadiene doped
!    methane flames: Flame modeling, Benzene, and Styrene Formation"
!Burcat 13-JAN-2011
FULVENE           T12/10C  6.H  6.   0.   0.G   200.000  6000.000 1000.
1
 1.14345282E+01 1.99371432E-02-7.13567060E-06 1.14951842E-09-
6.87263886E-14    2
 2.04411455E+04-3.86799524E+01 5.09714763E-01 2.58195980E-02
5.06504954E-05    3
-9.32593825E-08 4.15963672E-11 2.44318827E+04 2.30638077E+01
2.60142888E+04    4
!FULVENE    98 MARINOVC&FC   6H   6    0    0G   300.000  3000.000
1000.00      1
! 0.55099388E+01 0.33879936E-01-0.17737071E-04 0.44769284E-08-
0.44127372E-12    2
! 0.24921871E+05-0.67757489E+01-0.56096307E+01 0.73064757E-01-
0.70326923E-04    3
! 0.36580449E-07-0.80201931E-11 0.27468885E+05 0.48339178E+02
4
benzene                 C   6H   6O   0     G   300.000  5000.000
995.043    1
 1.27990377E+01 1.76655693E-02-5.86430896E-06 8.97294950E-10-
5.17334226E-14    2
 3.65624658E+03-4.90892144E+01 2.68313323E+00 2.29288793E-03
1.01785184E-04    3
-1.27824197E-07 4.65088580E-11 8.44358204E+03 1.36039292E+01
4
!Burcat 30-SEPT-2010
C6H5 phenyl radi  T07/10C  6.H  5.   0.   0.G   200.000  6000.000 1000.
1
 1.09540673E+01 1.82072569E-02-6.63331157E-06 1.08125690E-09-
6.51736617E-14    2
 3.51098413E+04-3.64320659E+01 4.91024498E-01 1.72669813E-02
7.02556406E-05    3
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-1.13389805E-07 4.89202543E-11 3.92340510E+04 2.42505364E+01
4.05676342E+04    4
!CBSQB3
C6H4                    C   6H   4O   0     G   300.000  5000.000
995.043    1
 1.21408245E+01 1.34649743E-02-4.54925841E-06 7.05803444E-10-
4.11247283E-14    2
 4.97703983E+04-4.22109775E+01 2.81396442E+00 9.27142960E-03
6.46141886E-05    3
-8.77361156E-08 3.27577572E-11 5.36902518E+04 1.31094297E+01
4
C6H5O                   C   6H   5O   1     G   300.000  5000.000
995.043    1
 1.48501937E+01 1.80685471E-02-7.27702186E-06 1.26940564E-09-
8.00651138E-14    2
-1.49781177E+03-5.56608868E+01 3.24731978E+00 1.99044110E-02
5.75005740E-05    3
-8.73852128E-08 3.35639730E-11 3.02944520E+03 1.14047946E+01
4
C5H5                    C   5H   5O   0     G   300.000  5000.000
995.043    1
 1.19820938E+01 1.21872945E-02-3.76158670E-06 5.45206715E-10-
3.01508977E-14    2
 2.65295823E+04-4.29105872E+01 2.66966211E+00 6.42151685E-03
7.00546223E-05    3
-9.25433638E-08 3.43204252E-11 3.05215272E+04 1.27169645E+01
4
C6H5OH             82489C   6H   6O   1     g  0300.00   4000.00
1000.00      1
 0.01821633e+03 0.01142427e+00-0.01096684e-04-0.06427442e-08
0.01198893e-11    2
-0.02053664e+06-0.07304234e+03 0.01391456e+02 0.03931958e+00
0.01777096e-04    3
-0.02277673e-06 0.08309659e-10-0.01472181e+06 0.01917813e+03
4
cyC5H6                  C   5H   6O   0     G   300.000  5000.000
995.043    1
 1.16960721E+01 1.59448522E-02-5.20901194E-06 7.87058917E-10-
4.49443430E-14    2
 1.05765973E+04-4.12952705E+01 2.73255616E+00 1.33819634E-03
9.31475596E-05    3
-1.16255819E-07 4.22115401E-11 1.48673400E+04 1.45010456E+01
4
C5H5CH3_1               C   6H   8O   0     G   300.000  5000.000
995.043    1
 1.44605240E+01 2.06645023E-02-6.77766039E-06 1.03031072E-09-
5.91870200E-14    2
 6.62751623E+03-5.52693435E+01 2.52788754E+00 1.37352012E-02
8.64247714E-05    3
-1.16860185E-07 4.34908216E-11 1.17199483E+04 1.58958041E+01
4
C5H5CH3_2               C   6H   8O   0     G   300.000  5000.000
995.043    1
 1.28114867E+01 2.28104249E-02-7.81703757E-06 1.22818027E-09-
7.23125298E-14    2
 5.72618641E+03-4.51979287E+01 2.79944630E+00 1.15409526E-02
8.68320938E-05    3
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-1.14217335E-07 4.20055902E-11 1.02690508E+04 1.58700657E+01
4
C5H5CH3_3               C   6H   8O   0     G   300.000  5000.000
995.043    1
 1.30104854E+01 2.25224745E-02-7.67174372E-06 1.20004642E-09-
7.04289314E-14    2
 5.49916395E+03-4.63690531E+01 2.76130849E+00 1.14294707E-02
8.78823752E-05    3
-1.15636361E-07 4.25540470E-11 1.01276765E+04 1.60350473E+01
4
!C8H6                    C   8H   6    0    0G   300.000  5000.000
1389.00      1
! 1.91822134e+01 1.76449850e-02-6.18210588e-06 9.75697439e-10-
5.72698125e-14    2
! 2.89847171e+04-8.01903000e+01-3.13527908e+00 7.15153321e-02-
5.60924468e-05    3
! 2.20854359e-08-3.49225990e-12 3.65086712e+04 3.89669546e+01
4
!Active Thermochemical Tables (17-DEC-2010)
C8H6  C6H5CCH     T12/06C  8.H  6.   0.   0.G   200.000  6000.000 1000.
1
 1.63582907E+01 2.11974105E-02-7.65817215E-06 1.24134505E-09-
7.45327960E-14    2
 3.10375340E+04-6.22520227E+01-2.74707918E+00 7.78284438E-02-
6.69709932E-05    3
 2.37972496E-08-8.43279765E-13 3.61131008E+04 3.54221257E+01
3.82082350E+04    4
C6H5CH3           mar95 C   7H   8    0    0g   300.000  5000.000
1389.000     1
 1.63091542e+01 2.25331612e-02-7.84281827e-06 1.23200630e-09-
7.20675043e-14    2
-2.66241940e+03-6.59814631e+01-4.08982289e+00 6.86477373e-02-
4.74716566e-05    3
 1.67001205e-08-2.39578007e-12 4.59499696e+03 4.41527734e+01
4
!Burcat 30-SEPT-2010
C6H5CH2     rad   T08/90C   7H   7    0    0G   200.000  6000.000 1000.
1
 0.14043980E+02 0.23493873E-01-0.85375367E-05 0.13890841E-08-
0.83614420E-13    2
 0.18564203E+05-0.51665589E+02 0.48111540E+00 0.38512832E-01
0.32861492E-04    3
-0.76972721E-07 0.35423068E-10 0.23307027E+05 0.23548820E+02
0.25317186E+05    4
C6H5C2H3                C   8H   80   00   0G   300.000  5000.000
1397.000     1
 2.00664002E+01 2.13200130E-02-7.39420054E-06 1.15900293E-09-
6.77014373E-14    2
 7.95082943E+03-8.51540631E+01-5.96522625E+00 8.73311719E-02-
7.23407283E-05    3
 3.04855159E-08-5.15901157E-12 1.64198720E+04 5.27226485E+01
4
!Burcat 30-SEPT-2010
C6H5CCH2          T12/07C  8.H  7.   0.   0.G   200.000  6000.000 1000.
1
 1.61678053E+01 2.34869894E-02-8.45465097E-06 1.36664033E-09-
8.19389188E-14    2
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 3.67356818E+04-5.98456163E+01 5.95576002E-01 4.31715811E-02
3.39695049E-05    3
-8.55153149E-08 4.02634981E-11 4.19756314E+04 2.57011560E+01
4.42221774E+04    4
!Burcat 13-JAN-2011
C5H4CH3           A03/05C  6.H  7.   0.   0.G   200.000  6000.000 1000.
1
 1.28996538E+01 2.12183240E-02-7.67565006E-06 1.24495899E-09-
7.47731827E-14    2
 2.12053775E+04-4.47534535E+01 5.64034275E-01 3.84201803E-02
1.94958520E-05    3
-5.95545053E-08 2.86869522E-11 2.53304225E+04 2.27464371E+01
2.72743433E+04    4
!C5H4CH3                C   6H   7O   0     G   300.000  5000.000
995.043    1
! 1.36818475E+01 1.90575918E-02-6.35439667E-06 9.78951164E-10-
5.68197013E-14    2
! 2.03302521E+04-4.83556513E+01 2.65912829E+00 1.56456975E-02
7.07292077E-05    3
!-9.88652457E-08 3.71383922E-11 2.48863905E+04 1.66392834E+01
4
C5H5CH2-1              C   6H   70   00   0G   300.000  5000.000
1398.000     1
 1.75854699E+01 1.58083012E-02-5.49671640E-06 8.63067187E-10-
5.04754347E-14    2
 3.08174859E+04-6.78115249E+01-3.42355668E+00 7.05975967E-02-
6.11471177E-05    3
 2.68157030E-08-4.69274460E-12 3.75067184E+04 4.29354487E+01
4
C5H5CH2-2              C   6H   70   00   0G   300.000  5000.000
1396.000     1
 1.52937914E+01 1.84305481E-02-6.35986836E-06 9.93248621E-10-
5.78637916E-14    2
 1.91962522E+04-5.97458894E+01-5.39417365E+00 7.51043847E-02-
6.77690358E-05    3
 3.16886723E-08-5.91960482E-12 2.56132529E+04 4.85135887E+01
4
C5H5CH2-3              C   6H   70   00   0G   300.000  5000.000
1397.000     1
 1.53787161E+01 1.83356361E-02-6.32188797E-06 9.86758405E-10-
5.74626535E-14    2
 2.21778975E+04-6.01469818E+01-5.34257890E+00 7.55933007E-02-
6.88888970E-05    3
 3.24825676E-08-6.10432744E-12 2.85588845E+04 4.81169777E+01
4
ME2CYBE                C   6H   6O   0     G   300.000  5000.000
995.043    1
 1.10469622E+01 2.12671617E-02-7.18107233E-06 1.10331635E-09-
6.36893079E-14    2
 2.49295229E+04-3.98345948E+01 2.75610508E+00-5.08653752E-03
1.22515931E-04    3
-1.46070604E-07 5.20577915E-11 2.95340792E+04 1.49694180E+01
4
c5h4chchch2            C   8H   80   00   0G   300.000  5000.000
1392.000     1
 1.91124085E+01 2.23573465E-02-7.79981638E-06 1.22709502E-09-
7.18532161E-14    2
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 2.34811472E+04-7.81135742E+01-7.11559661E+00 9.38484119E-02-
8.53806608E-05    3
 4.02612732E-08-7.59499392E-12 3.17035893E+04 5.93517892E+01
4
cyC6H7                  C   6H   70   00   0G   300.000  5000.000
1398.000     1
 1.51062049E+01 1.84668650E-02-6.34765376E-06 9.88961945E-10-
5.75240899E-14    2
 1.69429123E+04-6.01488002E+01-5.49906564E+00 7.15639115E-02-
5.97084788E-05    3
 2.56638736E-08-4.44379302E-12 2.35828506E+04 4.87214655E+01
4
C#CCCC#C                C   6H   6O   0     G   300.000  5000.000
995.043    1
 1.17384314E+01 1.83573254E-02-5.35666782E-06 7.29192207E-10-
3.82058667E-14    2
 4.50850746E+04-3.22188486E+01 2.36805012E+00 4.07007912E-02-
1.59371324E-05    3
-7.65988732E-09 5.95825562E-12 4.77085221E+04 1.67534631E+01
4
C*C*CC*C*C              C   6H   6O   0     G   300.000  5000.000
995.043    1
 1.51317236E+01 1.50144723E-02-4.90067905E-06 7.45116779E-10-
4.28886813E-14    2
 4.12134493E+04-5.30774674E+01 2.55749965E+00 3.56919817E-02
8.95669333E-06    3
-3.87074780E-08 1.74490521E-11 4.51945550E+04 1.49538788E+01
4
!CH3CCCH2                C   4H   50   00   0G   300.000  5000.000
1678.000     1
!-5.72844989E+00 4.53800905E-02-1.62861273E-05 2.61784277E-09-
1.55735959E-13    2
! 3.64135561E+04 5.47011215E+01 5.79092559E+00-1.26233816E-02
6.80832493E-05    3
!-4.51738347E-08 9.18508455E-12 3.57411849E+04 4.47042121E+00
4
!Estimated by RMG using Group Additivity
CH3CCCH2                C   4H   5          G   300.000  5000.000
995.043    1
 7.04689300E+00 1.55622754E-02-5.07615979E-06 7.58447227E-10-
4.29252290E-14    2
 3.29257091E+04-1.09242337E+01 3.54856004E+00 1.28419977E-02
2.43249896E-05    3
-3.58909345E-08 1.34239198E-11 3.44527742E+04 1.01108466E+01
4
C4H4-123           82489C   4H   4          g   300.00   4000.00
1000.00      1
 8.65692370E+00 1.11089843E-02-3.67007557E-06 5.61934414E-10-
3.25097422E-14    2
 3.56928579E+04-2.17244887E+01 3.05796958E+00 1.72821228E-02
1.16475279E-05    3
-2.61980847E-08 1.08357236E-11 3.76157331E+04 9.32272405E+00
4
C6H9                    C   6H   9O   0     G   300.000  5000.000
995.043    1
 1.36288339E+01 2.45055787E-02-8.07546311E-06 1.23042786E-09-
7.08589527E-14    2
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 1.27234636E+04-4.54653810E+01 2.56830777E+00 2.90638735E-02
4.52075606E-05    3
-7.47713655E-08 2.91501468E-11 1.69000816E+04 1.77668995E+01
4
C5H10_1                 C   5H  100   00   0G   300.000  5000.000
1386.000     1
 1.48559323E+01 2.17591025E-02-7.19194271E-06 1.09245029E-09-
6.25175564E-14    2
-1.01357366E+04-5.37935447E+01-1.03155314E+00 5.71908168E-02-
3.69342122E-05    3
 1.22979706E-08-1.66699878E-12-4.44795547E+03 3.21336978E+01
4
C5H9_1_4                C   5H   90   00   0G   300.000  5000.000
1386.000     1
 1.44005264E+01 1.97092525E-02-6.52672481E-06 9.92646930E-10-
5.68527283E-14    2
 1.49179297E+04-4.85075997E+01-2.58380960E-01 5.26374151E-02-
3.44775847E-05    3
 1.16929988E-08-1.62204571E-12 2.01435390E+04 3.06932604E+01
4
C5H8_CYC_1              C   5H   80   00   0G   300.000  5000.000
1390.000     1
 1.31885733E+01 1.93242410E-02-6.37805858E-06 9.69719676E-10-
5.55803454E-14    2
-2.80795505E+03-5.01996062E+01-5.40494068E+00 6.30369195E-02-
4.53166470E-05    3
 1.65992484E-08-2.44212443E-12 3.55686916E+03 4.94543473E+01
4
C5H7_CYC_1_2            C   5H   70   00   0G   300.000  5000.000
1397.000     1
 1.34371140E+01 1.66929165E-02-5.43076782E-06 8.17274811E-10-
4.65279058E-14    2
 1.34884647E+04-5.08315224E+01-5.04928694E+00 6.37056409E-02-
5.15076303E-05    3
 2.14163469E-08-3.57197034E-12 1.94507145E+04 4.69702347E+01
4
C5H9_CYC                C   5H   90   00   0G   300.000  5000.000
1379.000     1
 1.04168752E+01 2.49465214E-02-8.24607239E-06 1.24922484E-09-
7.13120153E-14    2
 7.57797065E+03-3.13941504E+01-3.77656906E+00 5.20633502E-02-
2.53273551E-05    3
 4.68183880E-09 6.16801914E-15 1.31180381E+04 4.69884349E+01
4

!RMG computed NASA-7 polynomials, for s-butanol chemistry
!Primary Thermo Library: sBuOH (Species ID: sBuOH)
sBuOH                   C   4H  10O   1     G   300.000  5000.000
995.043    1
 1.20855910E+01 2.46802133E-02-8.55828232E-06 1.35547557E-09-
8.03463474E-14    2
-4.10825366E+04-3.63567817E+01 3.44608509E+00 3.33125120E-02
1.77706231E-05    3
-4.26431467E-08 1.75965809E-11-3.80712117E+04 1.17730350E+01
4

!Primary Thermo Library: sBuOH-radicals (Species ID: CH3C[OH]C2H5)
```

```
CH3C[OH]C2H5            C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.11131685E+01 2.52738138E-02-8.98252392E-06 1.43738447E-09-
8.56524849E-14    2
-1.98180972E+04-3.20566125E+01 3.54087571E+00 2.43262516E-02
3.97619037E-05    3
-6.29219464E-08 2.40491096E-11-1.67572855E+04 1.22457012E+01
4

!Primary Thermo Library: sBuOH-radicals (Species ID: CH3CH[O]C2H5)
CH3CH[O]C2H5            C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.12336211E+01 2.51547674E-02-8.87271761E-06 1.41313903E-09-
8.39235232E-14    2
-1.42176960E+04-3.41023557E+01 3.50034101E+00 1.87537341E-02
5.72892014E-05    3
-8.07772664E-08 3.00788808E-11-1.08228318E+04 1.24934249E+01
4

!Primary Thermo Library: sBuOH-radicals (Species ID: CH3CH[OH]CHCH3)
CH3CH[OH]CHCH3          C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.17210637E+01 2.45991699E-02-8.69774819E-06 1.38693218E-09-
8.24492367E-14    2
-1.69857909E+04-3.41693245E+01 3.47587631E+00 2.80588967E-02
3.08366377E-05    3
-5.50824766E-08 2.16380379E-11-1.38753407E+04 1.29525071E+01
4

!Primary Thermo Library: sBuOH-radicals (Species ID: CH2CH[OH]C2H5)
CH2CH[OH]C2H5           C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.22910742E+01 2.36846497E-02-8.22921500E-06 1.29584781E-09-
7.63418132E-14    2
-1.62241282E+04-3.88217489E+01 3.35701560E+00 2.74981490E-02
3.44130786E-05    3
-5.96953887E-08 2.33931643E-11-1.28570092E+04 1.22209313E+01
4

!Primary Thermo Library: sBuOH-radicals (Species ID: CH3CH[OH]CH2CH2)
CH3CH[OH]CH2CH2         C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.21482917E+01 2.42621454E-02-8.57620180E-06 1.36698770E-09-
8.12357664E-14    2
-1.63752860E+04-3.74122557E+01 3.44210435E+00 2.97543713E-02
2.76239378E-05    3
-5.26874125E-08 2.09869899E-11-1.31819698E+04 1.18867373E+01
4

!CH3CH[OH]CH2            C   3H   7O   1     G   300.000  5000.000
995.043    1
! 9.77349379E+00 1.64188798E-02-5.42302225E-06 8.35595432E-10-
4.86468599E-14    2
!-1.27504154E+04-2.31244729E+01 2.98550534E+00 1.99464635E-02
2.50762522E-05    3
!-4.35955166E-08 1.71435984E-11-1.02233146E+04 1.55003786E+01
4
```

```
!HOCHC2H5                C   3H   7O   1     G   300.000  5000.000
995.043    1
! 1.06227801E+01 1.58439620E-02-6.29817026E-06 1.10707477E-09-
7.04376940E-14    2
!-1.35923367E+04-2.78896852E+01 3.58171453E+00 2.27311779E-02
1.56056258E-05    3
!-3.51994938E-08 1.44861872E-11-1.11308272E+04 1.13721922E+01
4

H2CCCH3[OH]              C   3H   6O   1     G   300.000  5000.000
995.043    1
 8.29437947E+00 1.58753727E-02-5.64467607E-06 9.18221350E-10-
5.55545783E-14    2
-2.32857423E+04-1.66761815E+01 3.31481341E+00 1.83931001E-02
1.69403436E-05    3
-3.18880367E-08 1.26275245E-11-2.14284312E+04 1.16758545E+01
4

CH3CH-O-CH3              C   3H   7O   1     G   300.000  5000.000
995.043    1
 1.18175293E+01 1.43160787E-02-5.48284569E-06 9.44520573E-10-
5.93743616E-14    2
-9.27581460E+03-3.58250415E+01 3.33540219E+00 2.14317612E-02
2.44648704E-05    3
-4.63714556E-08 1.86753336E-11-6.25204835E+03 1.17661912E+01
4

CH3C[OH]CH3              C   3H   7O   1     G   300.000  5000.000
995.043    1
 9.37394265E+00 1.69531922E-02-5.67677769E-06 8.84041426E-10-
5.18941694E-14    2
-1.57647444E+04-2.18338538E+01 3.05848782E+00 2.59725170E-02
5.40167360E-06    3
-2.30702320E-08 1.01200600E-11-1.36975915E+04 1.26749814E+01
4

acetone                  C   3H   6O   1     G   300.000  5000.000
995.043    1
 7.35982543E+00 1.78808265E-02-6.80770588E-06 1.15402665E-09-
7.16532052E-14    2
-2.95584158E+04-1.32906679E+01 3.61211380E+00 1.17333498E-02
3.44374804E-05    3
-4.79046469E-08 1.76370250E-11-2.77624285E+04 1.00482121E+01
4

C2H5CHCHCH2              C   5H   9          G   300.000  5000.000
995.043    1
 1.21965725E+01 2.28772985E-02-7.83515339E-06 1.23415177E-09-
7.28951410E-14    2
 8.28497139E+03-3.84961951E+01 2.87980231E+00 2.34129716E-02
4.70088143E-05    3
-7.27964666E-08 2.78948571E-11 1.19666866E+04 1.55890510E+01
4

CH2C[OH]CH2              C   3H   5O   1     G   300.000  5000.000
995.043    1
```

```
 9.56877928E+00 1.22119232E-02-4.20019790E-06 6.67391525E-10-
3.97143096E-14    2
-5.48793134E+03-2.41197985E+01 3.10981530E+00 1.72614775E-02
1.97165518E-05    3
-3.64804691E-08 1.46008088E-11-3.16713391E+03 1.22117043E+01
4

CH2C[O]CH3              C   3H   5O   1     G   300.000  5000.000
995.043    1
 6.79706896E+00 1.57806872E-02-5.82778600E-06 9.68387957E-10-
5.93768966E-14    2
-4.56818488E+03-8.19716766E+00 3.50742664E+00 1.69701545E-02
1.05210431E-05    3
-2.21399974E-08 8.80035584E-12-3.31773613E+03 1.06508565E+01
4

CH3-O-C(CH3)2           C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.01721325E+01 2.44515310E-02-8.51235884E-06 1.36047918E-09-
8.13061068E-14    2
-1.32663328E+04-2.38376502E+01 3.13909453E+00 3.63540713E-02-
1.77814055E-06    3
-1.96846417E-08 9.36009617E-12-1.10563046E+04 1.41298954E+01
4

C4H7O_1_2               C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.22647725E+01 1.72544362E-02-5.82185308E-06 9.09555514E-10-
5.34309894E-14    2
-9.96864505E+03-3.85927049E+01 2.85054465E+00 2.14634434E-02
3.85377986E-05    3
-6.27823578E-08 2.44840555E-11-6.42999031E+03 1.51459104E+01
4

C3H6O-enol              C   3H   6O   1     G   300.000  5000.000
995.043    1
 9.64710700E+00 1.42646816E-02-4.77427505E-06 7.43381932E-10-
4.36053046E-14    2
-2.31642975E+04-2.49946208E+01 3.03862899E+00 1.74444519E-02
2.56858167E-05    3
-4.32839387E-08 1.69523341E-11-2.06914263E+04 1.26721005E+01
4

MEK                     C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.00246517E+01 2.26795049E-02-8.38430069E-06 1.39637667E-09-
8.57605820E-14    2
-3.33778012E+04-2.46743054E+01 3.40612649E+00 2.61007797E-02
2.14085539E-05    3
-4.19807790E-08 1.66957938E-11-3.09128868E+04 1.29908086E+01
4

sC4H8O                  C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.30086754E+01 1.84993987E-02-6.41762267E-06 1.02768177E-09-
6.14948415E-14    2
```

```
-2.56748322E+04-4.12083327E+01 2.92775149E+00 2.31555495E-02
4.06340482E-05    3
-6.67230823E-08 2.60623760E-11-2.18929571E+04 1.62988569E+01
4

CH3CH(O)C2H5            C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.23095478E+01 2.24197258E-02-7.64690634E-06 1.20290614E-09-
7.10238644E-14    2
-1.50659395E+04-3.77344493E+01 2.87489217E+00 2.77459011E-02
3.34683351E-05    3
-5.92699028E-08 2.33950280E-11-1.15744601E+04 1.58451370E+01
4

C4H7O(337)              C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.11944529E+01 1.85295495E-02-6.55565804E-06 1.06114030E-09-
6.39566758E-14    2
-1.03186178E+04-3.11423061E+01 3.10445637E+00 2.74552100E-02
1.55587884E-05    3
-3.75865006E-08 1.56335768E-11-7.54053004E+03 1.37166902E+01
4

C4H6O(717)              C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.05344019E+01 1.73239907E-02-6.42390590E-06 1.07118475E-09-
6.57978651E-14    2
-2.01330910E+04-2.85513388E+01 3.28295365E+00 1.83743856E-02
3.43524931E-05    3
-5.46290937E-08 2.10591384E-11-1.72988909E+04 1.33868218E+01
4

C4H7O(238)              C   4H   7O   1     G   300.000  5000.000
995.043    1
 8.42274260E+00 2.20983135E-02-8.18324614E-06 1.36213673E-09-
8.36192628E-14    2
-9.39887129E+03-1.52196753E+01 3.50206771E+00 2.71638869E-02
6.36327972E-06    3
-2.32460289E-08 9.83312382E-12-7.69113226E+03 1.21558424E+01
4

cH2C[O]C2H5             C   4H   7O   1     G   300.000  5000.000
995.043    1
 9.76241174E+00 2.04773296E-02-7.68086635E-06 1.28311441E-09-
7.88457698E-14    2
-8.44832738E+03-2.05964529E+01 3.91741832E+00 2.36779609E-02
1.80896664E-05    3
-3.64813794E-08 1.45594800E-11-6.28036886E+03 1.26220168E+01
4

CH3C[O]cHCH3            C   4H   7O   1     G   300.000  5000.000
995.043    1
 8.44947961E+00 2.21126871E-02-8.20349004E-06 1.36033796E-09-
8.32012183E-14    2
-9.43240451E+03-1.54289887E+01 3.98549677E+00 2.37988791E-02
1.37641647E-05    3
```

```
-2.97788246E-08 1.18660994E-11-7.73913874E+03 1.01294886E+01
4

CH3C[O]CH2cH2           C   4H   7O   1     G   300.000  5000.000
995.043    1
 9.76241174E+00 2.04773296E-02-7.68086635E-06 1.28311441E-09-
7.88457698E-14    2
-8.44832738E+03-2.05964529E+01 3.91741832E+00 2.36779609E-02
1.80896664E-05    3
-3.64813794E-08 1.45594800E-11-6.28036886E+03 1.26220168E+01
4

MEKenol2                C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.12046688E+01 2.06883401E-02-7.29961446E-06 1.17134589E-09-
7.00592872E-14    2
-2.71249127E+04-3.05719589E+01 3.57566103E+00 2.28780180E-02
3.23298931E-05    3
-5.41427886E-08 2.10539010E-11-2.41968382E+04 1.32799826E+01
4

CH2C[OH]cHCH3           C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.11873120E+01 1.86172946E-02-6.61927097E-06 1.06604474E-09-
6.38975583E-14    2
-1.03425902E+04-3.11730045E+01 3.58128206E+00 2.41087870E-02
2.29162011E-05    3
-4.40571208E-08 1.76383366E-11-7.58711923E+03 1.17238573E+01
4

CH2C[OH]CH2cH2          C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.09495697E+01 1.83984198E-02-6.53256718E-06 1.05317919E-09-
6.32035925E-14    2
-2.17146651E+03-2.64634081E+01 3.61012717E+00 2.38016221E-02
2.16535928E-05    3
-4.21727688E-08 1.69128275E-11 4.82268910E+02 1.49040237E+01
4

cHC[OH]C2H5             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.14112794E+01 1.78712191E-02-6.29560832E-06 1.00967841E-09-
6.03801873E-14    2
 2.79697073E+03-2.99657675E+01 3.55104417E+00 2.61167736E-02
1.64769828E-05    3
-3.78329611E-08 1.56243519E-11 5.51727850E+03 1.37253275E+01
4

MEKenol                 C   4H   8O   1     G   300.000  5000.000
995.043    1
 9.91291222E+00 2.22807440E-02-8.06374915E-06 1.31687456E-09-
7.97378270E-14    2
-2.81404012E+04-2.37293875E+01 3.78628018E+00 2.52404096E-02
2.01399928E-05    3
-3.94646884E-08 1.56650523E-11-2.58484165E+04 1.11880075E+01
4
```

```
CH3C[OH]cCH3            C   4H   7O   1     G   300.000  5000.000
995.043    1
 9.15923628E+00 2.06093801E-02-7.58087453E-06 1.25183792E-09-
7.63886679E-14    2
 1.05022250E+03-1.74398559E+01 3.89725222E+00 2.90106097E-02-
1.02286066E-06    3
-1.60208891E-08 7.49908058E-12 2.72867507E+03 1.10921142E+01
4

CH3C[OH]CHcH2           C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.11873120E+01 1.86172946E-02-6.61927097E-06 1.06604474E-09-
6.38975583E-14    2
-1.03425902E+04-3.11730045E+01 3.58128206E+00 2.41087870E-02
2.29162011E-05    3
-4.40571208E-08 1.76383366E-11-7.58711923E+03 1.17238573E+01
4

cH2CH[OH]C2H3           C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.27464354E+01 1.62972234E-02-5.71418833E-06 9.14419508E-10-
5.45800294E-14    2
-7.45358402E+02-3.71304802E+01 3.43904333E+00 2.07327306E-02
3.73151606E-05    3
-6.12236827E-08 2.39260622E-11 2.73956088E+03 1.59300651E+01
4

CH3CH[OH]cCH2           C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.22478586E+01 1.69157798E-02-5.99836098E-06 9.67549556E-10-
5.80865649E-14    2
 3.49181904E+03-3.49494994E+01 3.51554922E+00 2.35793266E-02
2.68286073E-05    3
-4.97499033E-08 1.99011640E-11 6.63754532E+03 1.42101307E+01
4

CH3CH[OH]CHcH           C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.32081452E+01 1.57700227E-02-5.47722947E-06 8.70918728E-10-
5.17566242E-14    2
 4.22307884E+03-4.06328396E+01 3.37996033E+00 2.30478821E-02
3.21385506E-05    3
-5.68838751E-08 2.26375866E-11 7.77457047E+03 1.47513689E+01
4

CH3CH[o]C2H3            C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.29328889E+01 1.67583588E-02-5.91936607E-06 9.51231590E-10-
5.69195899E-14    2
 5.65895120E+02-4.10141088E+01 3.44097576E+00 1.82030196E-02
4.72454073E-05    3
-7.17473741E-08 2.75241695E-11 4.27232029E+03 1.38642529E+01
4

CH3CHcOH                C   3H   5O   1     G   300.000  5000.000
995.043    1
```

```
 9.88045468E+00 1.14619342E-02-3.79051281E-06 5.79915686E-10-
3.35081601E-14    2
 6.72405274E+03-2.45977428E+01 3.49744119E+00 1.73181998E-02
1.72337915E-05    3
-3.35069070E-08 1.35557606E-11 8.97468394E+03 1.10910916E+01
4

CH3C[OH]cH              C   3H   5O   1     G   300.000  5000.000
995.043    1
 8.52772715E+00 1.30726253E-02-4.66091383E-06 7.54755105E-10-
4.54574338E-14    2
 6.60260793E+03-1.62793035E+01 3.77362561E+00 1.82668480E-02
8.48831830E-06    3
-2.21110049E-08 9.23095105E-12 8.23767907E+03 1.00948456E+01
4


!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!
! New work for sec- and tert-butanol paper:
!
!    "Accurate Reaction Networks for Alternative Fuels: Butanol Isomers"
!
!    K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
!
!    To be submitted to Industrial & Engineering Chemical Research
!
!       for the ISCRE-21 conference
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!

!Primary Thermo Library: MRH (Species ID: HOCHCH2CH3)
HOCHC2H5                C   3H   7O   1     G   300.000  5000.000
995.043    1
 9.59294739E+00 1.66880281E-02-5.66970089E-06 8.84284576E-10-
5.18176412E-14    2
-1.34935100E+04-2.23802574E+01 3.54748101E+00 1.62026450E-02
3.24288177E-05    3
-4.96765804E-08 1.89413813E-11-1.10632817E+04 1.29217907E+01
4

!Primary Thermo Library: MRH (Species ID: HOCH[CH3]CH2)
CH3CH[OH]CH2            C   3H   7O   1     G   300.000  5000.000
995.043    1
 1.03366849E+01 1.57197410E-02-5.23359759E-06 8.05258237E-10-
4.67634710E-14    2
-1.18433438E+04-2.64605633E+01 3.45943591E+00 2.67857923E-02
3.07851910E-06    3
-2.15093640E-08 9.76694186E-12-9.65391150E+03 1.08084614E+01
4

!Primary Thermo Library: MRH (Species ID: HOCHCH3)
C2H5O-2                 C   2H   5O   1     G   300.000  5000.000
995.043    1
 6.95952386E+00 1.17750088E-02-4.03080988E-06 6.32485588E-10-
3.72303902E-14    2
```

```
-9.79839142E+03-1.00096844E+01 3.76833687E+00 8.00813773E-03
2.66644779E-05    3
-3.66939631E-08 1.35519905E-11-8.34176353E+03 9.49832589E+00
4

!Primary Thermo Library: MRH (Species ID: C4H5-113)
!C4H5-113               C   4H   5          G   300.000  5000.000
995.043    1
! 9.02577751E+00 1.39818587E-02-5.07003487E-06 8.25067458E-10-
4.98015293E-14    2
! 3.53944834E+04-1.83669800E+01 3.74950555E+00 2.68190415E-02-
1.17995959E-05    3
!-3.12289209E-09 3.06680917E-12 3.68590187E+04 9.14464700E+00
4

!Primary Thermo Library: MRH (Species ID: C4H7-14)
C4H7-14                 C   4H   7          G   300.000  5000.000
995.043    1
 8.97000250E+00 1.79258195E-02-6.17424562E-06 9.72336791E-10-
5.73787633E-14    2
 2.12362140E+04-1.96846722E+01 3.62922367E+00 1.63308301E-02
3.09993172E-05    3
-4.72284199E-08 1.79055863E-11 2.34408961E+04 1.17925067E+01
4

!Primary Thermo Library: tBuOH_species_MRH (Species ID: tBuOH)
tBuOH                   C   4H  10O   1     G   300.000  5000.000
995.043    1
 1.32888966E+01 2.28710143E-02-7.63003530E-06 1.17452119E-09-
6.81884393E-14    2
-4.42603655E+04-4.62525045E+01 3.20127219E+00 3.19490409E-02
2.61305244E-05    3
-5.32325188E-08 2.15878935E-11-4.06947307E+04 1.01936894E+01
4

iC4H8                   C   4H   8          G   300.000  5000.000
995.043    1
 8.71463774E+00 2.11044876E-02-7.36931915E-06 1.17117674E-09-
6.95538926E-14    2
-6.19698532E+03-2.23043825E+01 3.68975963E+00 1.67587430E-02
3.61832844E-05    3
-5.27991092E-08 1.97187543E-11-3.98185957E+03 8.01870691E+00
4

HOC[CH2][CH3]2          C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.26392838E+01 2.14980270E-02-7.31826790E-06 1.14214079E-09-
6.69476785E-14    2
-1.89368121E+04-3.87206289E+01 3.31715236E+00 2.73287028E-02
3.15940430E-05    3
-5.68883342E-08 2.25426759E-11-1.55150949E+04 1.40786285E+01
4

!Primary Thermo Library: tBuOH_species_MRH (Species ID: OC[CH3]3)
OC[CH3]3                C   4H   9O   1     G   300.000  5000.000
995.043    1
```

```
 1.27020516E+01 2.15518290E-02-7.22660324E-06 1.11589980E-09-
6.49265761E-14    2
-1.63678834E+04-4.23206612E+01 3.26391102E+00 3.12339305E-02
2.07768752E-05    3
-4.61868988E-08 1.89904362E-11-1.30906593E+04 1.01956220E+01
4
iC4H7                   C   4H   7          G   300.000  5000.000
995.043    1
 8.34970451E+00 1.92508033E-02-6.81360221E-06 1.08484853E-09-
6.42422082E-14    2
 1.24406647E+04-1.87060633E+01 2.38739541E+00 2.06784631E-02
2.89299685E-05    3
-5.37553477E-08 2.35670326E-11 1.47584145E+04 1.55529104E+01
1.65497991E+04    4

HCC[CH3]2               C   4H   7          G   300.000  5000.000
995.043    1
 8.92124841E+00 1.82873666E-02-6.36531302E-06 1.00950927E-09-
5.98747927E-14    2
 2.37248981E+04-2.10051137E+01 3.66514278E+00 1.99974987E-02
2.03303741E-05    3
-3.64892818E-08 1.42892052E-11 2.57322572E+04 9.15712920E+00
4

iC4H10                  C   4H  10          G   300.000  5000.000
995.043    1
 9.90138526E+00 2.46640732E-02-8.42860567E-06 1.31706206E-09-
7.72354421E-14    2
-2.14932759E+04-3.06727543E+01 3.49480838E+00 1.42425382E-02
6.18151770E-05    3
-8.22822811E-08 3.01064414E-11-1.84274253E+04 9.20248321E+00
4

tC4H9                   C   4H   9          G   300.000  5000.000
995.043    1
 6.51964415E+00 2.61732410E-02-9.41585548E-06 1.52671032E-09-
9.19528715E-14    2
 2.42927323E+03-8.39699210E+00 3.99209760E+00 1.92505813E-02
2.67723481E-05    3
-3.99728022E-08 1.46695645E-11 3.77798978E+03 8.03403035E+00
4

iC4H9                   C   4H   9          G   300.000  5000.000
995.043    1
 8.95092770E+00 2.30274814E-02-7.50785505E-06 1.12742662E-09-
6.41369663E-14    2
 3.75692818E+03-2.12760459E+01 3.34836782E+00 1.76633897E-02
4.26157222E-05    3
-6.06192866E-08 2.25256541E-11 6.25239496E+03 1.26621599E+01
4



sSPC(116)               C   4H   9O   3     G   300.000  5000.000
995.043    1
```

```
 1.60487784E+01 2.34687220E-02-7.72308455E-06 1.17145286E-09-
6.72081120E-14    2
-3.62942866E+04-5.05625934E+01 2.91112461E+00 4.74936895E-02-
5.43770406E-07    3
-3.27135996E-08 1.57512201E-11-3.22546437E+04 1.99148898E+01
4

sSPC(46)               C   4H   7O   2     G   300.000  5000.000
995.043    1
 1.38671524E+01 1.84946231E-02-6.36934628E-06 1.00248981E-09-
5.91132591E-14    2
 5.31284989E+02-4.19913964E+01 3.27948470E+00 3.13280470E-02
1.90991226E-05    3
-4.60862571E-08 1.93154122E-11 4.11003276E+03 1.64305806E+01
4

sSPC(56)               C   4H   7O   2     G   300.000  5000.000
995.043    1
 1.05403877E+01 2.26686073E-02-8.15961393E-06 1.32318495E-09-
7.96965901E-14    2
 2.62225552E+03-2.24439816E+01 3.68861124E+00 3.40054561E-02-
8.18299033E-07    3
-1.99640888E-08 9.38119187E-12 4.78814336E+03 1.46094431E+01
4

sSPC(752)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.48140311E+01 2.09509218E-02-7.88757522E-06 1.32020695E-09-
8.11961743E-14    2
-2.82110013E+04-4.42453804E+01 3.57885771E+00 3.65604607E-02
1.31348980E-05    3
-4.26148575E-08 1.84570333E-11-2.45119682E+04 1.72541366E+01
4

sSPC(332)              C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.60970130E+01 2.38091870E-02-8.99834681E-06 1.51505047E-09-
9.36198290E-14    2
-3.41213906E+04-4.98936494E+01 3.59977440E+00 4.41622210E-02
5.37077503E-06    3
-3.82955599E-08 1.74920770E-11-3.01548630E+04 1.77704009E+01
4

sSPC(1013)             C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.74871930E+01 2.29177950E-02-8.98184496E-06 1.54554884E-09-
9.68175821E-14    2
-3.12599605E+04-5.64279702E+01 3.65727383E+00 5.28629793E-02-
1.54565824E-05    3
-2.00227555E-08 1.18309623E-11-2.72378675E+04 1.66054011E+01
4

sSPC(1072)             C   4H   8O   3     G   300.000  5000.000
995.043    1
 1.57883015E+01 2.31043970E-02-9.67066160E-06 1.72738546E-09-
1.10646551E-13    2
```

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-4.52462396E+04-4.92351514E+01 4.11745810E+00 4.26620933E-02
2.08846171E-06    3
-3.37826077E-08 1.57533738E-11-4.15692579E+04 1.38175802E+01
4

sSPC(1151)              C   4H   7O   2     G   300.000  5000.000
995.043    1
 1.28092078E+01 2.05039167E-02-8.72389141E-06 1.57590816E-09-
1.01646743E-13    2
-2.61339424E+04-3.56312957E+01 4.32889836E+00 2.77859653E-02
2.07112251E-05    3
-4.52212247E-08 1.84586338E-11-2.31191357E+04 1.19079738E+01
4

sSPC(1356)              C   3H   5O   3     G   300.000  5000.000
995.043    1
 1.30620218E+01 1.36065903E-02-4.50253652E-06 6.86701019E-10-
3.95108324E-14    2
-2.20276347E+04-3.60092157E+01 3.23105491E+00 1.67354145E-02
4.56392187E-05    3
-6.96621191E-08 2.68697013E-11-1.82696357E+04 2.04232998E+01
4

sSPC(1697)              C   1H   3O   2     G   300.000  5000.000
995.043    1
 4.50709758E+00 1.00591648E-02-3.50669922E-06 5.54663429E-10-
3.28240922E-14    2
 2.76115385E+02 3.79532293E+00 3.95829613E+00 8.12808570E-03
5.64109904E-06    3
-9.75279769E-09 3.60671985E-12 5.90146803E+02 7.46942342E+00
4

sSPC(1735)              C   1H   4O   2     G   300.000  5000.000
995.043    1
 6.55192777E+00 1.09233807E-02-4.00348919E-06 6.54882510E-10-
3.96302306E-14    2
-1.88015717E+04-8.83124515E+00 3.90834693E+00 9.87918630E-03
1.51646204E-05    3
-2.39752977E-08 9.11021710E-12-1.76976879E+04 6.81270224E+00
4

sSPC(1909)              C   2H   2O   2     G   300.000  5000.000
995.043    1
 8.01192522E+00 6.65856648E-03-3.12847913E-06 5.95070011E-10-
3.94869481E-14    2
-4.41692307E+03-1.51118041E+01 4.20145012E+00 5.43189921E-03
2.36610759E-05    3
-3.40633679E-08 1.28665403E-11-2.83956199E+03 7.36822093E+00
4

sSPC(3071)              C   1H   1O   3     G   300.000  5000.000
995.043    1
 8.20784567E+00 3.85483955E-03-1.74687304E-06 3.26011598E-10-
2.13956681E-14    2
-1.58535388E+04-1.26938939E+01 3.94137227E+00 8.40452589E-03
1.03906079E-05    3
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-2.05330518E-08 8.41697543E-12-1.43806439E+04 1.10028618E+01
4

sSPC(3121)              C   1H   2O   3     G   300.000  5000.000
995.043    1
 1.02526759E+01 4.71905548E-03-2.24366302E-06 4.26230679E-10-
2.82018065E-14    2
-4.00288507E+04-2.53204620E+01 3.89142307E+00 1.01556265E-02
1.99141292E-05    3
-3.47555518E-08 1.39204727E-11-3.77661034E+04 1.03461406E+01
4

!sSPC(2810)              C   1H   1O   2     G   300.000  5000.000
995.043    1
! 6.33586637E+00 3.43117948E-03-2.37139468E-06 5.19512848E-10-
3.68906227E-14    2
!-2.17926651E+04-7.88494751E+00 4.53163202E+00-6.01162662E-03
3.70316909E-05    3
!-4.27425448E-08 1.50691240E-11-2.06070781E+04 4.96370739E+00
4
!Primary Thermo Library: Franklin (Species ID: formyloxy)
sSPC(2810)              C   1H   1O   2     G   300.000  5000.000
995.043    1
 5.61540843E+00 3.85579995E-03-1.36009488E-06 2.16777767E-10-
1.28581019E-14    2
-1.70993890E+04-3.88589948E+00 3.88443478E+00-2.82937050E-03
2.92849139E-05    3
-3.40948488E-08 1.20699055E-11-1.60794792E+04 7.85042689E+00
4

sSPC(1474)              C   3H   6O   3     G   300.000  5000.000
995.043    1
 1.51068520E+01 1.44708062E-02-4.99932650E-06 7.86920100E-10-
4.63169708E-14    2
-4.11053218E+04-4.86357838E+01 3.18110571E+00 1.84865151E-02
5.51627400E-05    3
-8.38846191E-08 3.23731985E-11-3.65574704E+04 1.97665786E+01
4

sSPC(1590)              C   3H   5O   2     G   300.000  5000.000
995.043    1
 1.21277583E+01 1.18703259E-02-4.05255631E-06 6.35442800E-10-
3.73171632E-14    2
-2.19930246E+04-3.50319282E+01 3.39254597E+00 3.61038707E-03
7.37855034E-05    3
-9.53232361E-08 3.50784586E-11-1.81073482E+04 1.78569722E+01
4



tSPC(54)                C   4H   7O   2     G   300.000  5000.000
995.043    1
 1.12235460E+01 2.19431957E-02-7.82038307E-06 1.25939897E-09-
7.54969440E-14    2
 2.15644501E+03-2.66584741E+01 3.59416332E+00 3.74159535E-02-
8.23636896E-06    3
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-1.38104998E-08 7.56701446E-12 4.42708313E+03 1.38913409E+01
4

tSPC(77)                C   4H   7O   2     G   300.000  5000.000
995.043    1
 1.45427760E+01 1.91439622E-02-6.87269486E-06 1.10878822E-09-
6.64628137E-14    2
 8.76568886E+02-4.67286592E+01 3.33921601E+00 3.80354315E-02
4.06336061E-06    3
-3.26254322E-08 1.50437960E-11 4.40054569E+03 1.37704695E+01
4

tSPC(122)               C   4H   7O   4     G   300.000  5000.000
995.043    1
 1.57772844E+01 2.36461198E-02-8.76823696E-06 1.44784027E-09-
8.82461338E-14    2
-8.56781176E+03-4.43322113E+01 3.44861781E+00 5.98242646E-02-
4.31325009E-05    3
 1.09556096E-08 9.18771859E-13-5.45180890E+03 1.84141763E+01
4

tSPC(157)               C   4H   7O   4     G   300.000  5000.000
995.043    1
 2.04964520E+01 1.84402229E-02-6.63312047E-06 1.07113314E-09-
6.42390379E-14    2
-1.06278634E+04-7.27578113E+01 2.92382617E+00 6.14395438E-02-
2.97848238E-05    3
-1.13349689E-08 1.00668747E-11-5.76236080E+03 1.88087075E+01
4

tSPC(213)               C   4H   6O   3     G   300.000  5000.000
995.043    1
 1.71062230E+01 1.67731762E-02-6.67823623E-06 1.15678179E-09-
7.26916988E-14    2
-2.98959697E+04-5.83539016E+01 3.55006185E+00 4.43261212E-02-
7.59945662E-06    3
-2.54369669E-08 1.34454970E-11-2.58644081E+04 1.36814431E+01
4

tSPC(97)                C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.66203434E+01 2.32608784E-02-8.81127317E-06 1.48619276E-09-
9.19423211E-14    2
-3.66570373E+04-5.47327594E+01 3.56714133E+00 4.45617347E-02
6.06931701E-06    3
-3.99670625E-08 1.82330725E-11-3.25161492E+04 1.59309131E+01
4

tSPC(439)               C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.84100745E+01 2.18351740E-02-8.54101587E-06 1.46824514E-09-
9.18927648E-14    2
-3.07812782E+04-6.32507766E+01 3.55165828E+00 4.72364394E-02
4.91653815E-06    3
-4.22195427E-08 1.95954962E-11-2.61248768E+04 1.68982330E+01
4
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!Primary Thermo Library: MRH (Species ID: tSPC(343))
tSPC(343)               C   4H   5O   2     G   300.000  5000.000
995.043    1
 1.46587694E+01 1.44038978E-02-5.32453345E-06 8.76472959E-10-
5.32275743E-14    2
-9.40029488E+03-4.96885296E+01 3.39013921E+00 2.83395380E-02
2.09473994E-05    3
-4.84021222E-08 2.02864286E-11-5.60507817E+03 1.24220877E+01
4

!Primary Thermo Library: Franklin (Species ID: CH2CCHO)
tSPC(346)               C   3H   3O   1     G   300.000  5000.000
995.043    1
 7.77376639E+00 1.00911203E-02-3.64332283E-06 5.89866784E-10-
3.54379966E-14    2
 2.01399452E+04-1.29618034E+01 3.78480317E+00 1.21631402E-02
1.42824953E-05    3
-2.55230139E-08 1.00685696E-11 2.16250444E+04 9.73634101E+00
4

tSPC(878)               C   3H   3O   3     G   300.000  5000.000
995.043    1
 1.20076040E+01 1.07771863E-02-4.44943376E-06 7.90916946E-10-
5.05604974E-14    2
-3.57538533E+03-3.01422827E+01 3.86586286E+00 3.38732169E-02-
2.47443161E-05    3
 4.65884103E-09 1.42210944E-12-1.47821374E+03 1.14928076E+01
4

!Primary Thermo Library: Franklin (Species ID: CH2CCO)
H2CCCO                  C   3H   2O   1     G   300.000  5000.000
995.043    1
 7.10621302E+00 7.85760609E-03-2.77708384E-06 4.44956861E-10-
2.65746406E-14    2
 1.38261399E+04-1.02916646E+01 3.80672140E+00 1.21373403E-02
4.31444438E-06    3
-1.33800030E-08 5.72661551E-12 1.49275237E+04 7.84494018E+00
4

!Primary Thermo Library: MRH (Species ID: tSPC(1286))
tSPC(1286)              C   3H   3O   3     G   300.000  5000.000
995.043    1
 1.27917510E+01 1.07507802E-02-4.11340474E-06 6.92704583E-10-
4.27125593E-14    2
-1.06730612E+04-3.78182619E+01 3.56608757E+00 2.60115259E-02
5.78316714E-06    3
-2.79816432E-08 1.26999837E-11-7.75658025E+03 1.20737734E+01
4

tSPC(1416)              C   3H   4O   3     G   300.000  5000.000
995.043    1
 1.53109429E+01 9.62329710E-03-3.35217132E-06 5.31082949E-10-
3.14073851E-14    2
-3.68903334E+04-4.96941549E+01 3.19820064E+00 2.76343182E-02
1.57479708E-05    3
-4.32535741E-08 1.87548324E-11-3.29608994E+04 1.63149381E+01
4
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!Primary Thermo Library: MRH (Species ID: tSPC[1553])
tSPC(1553)              C   3H   3O   2     G   300.000  5000.000
995.043    1
 1.08281746E+01 9.26775880E-03-3.24511635E-06 5.15798412E-10-
3.05787304E-14    2
-1.42268828E+04-2.96992226E+01 3.51998927E+00 1.29819235E-02
2.98439846E-05    3
-4.75740633E-08 1.85642059E-11-1.15019716E+04 1.19064760E+01
4

C8H14                   C   8H  14          G   300.000  5000.000
995.043    1
 1.83366365E+01 3.77743153E-02-1.33356362E-05 2.13641623E-09-
1.27596995E-13    2
-7.07395315E+03-6.65713995E+01 3.11484372E+00 5.38392334E-02
3.04725354E-05    3
-7.27908627E-08 3.01483905E-11-1.81072107E+03 1.80147789E+01
4

tSPC(3683)              C   3H   5O   3     G   300.000  5000.000
995.043    1
 1.14114223E+01 1.74246134E-02-6.75251474E-06 1.14832728E-09-
7.13491148E-14    2
-1.53355356E+04-2.62588332E+01 3.85191355E+00 3.59948729E-02-
1.69307314E-05    3
-3.96885918E-09 4.21330472E-12-1.32460519E+04 1.31138173E+01
4

C4H8O2(62)              C   4H   8O   2     G   300.000  5000.000
995.043    1
 1.32683761E+01 2.28074117E-02-8.31717304E-06 1.35961805E-09-
8.23030824E-14    2
-1.69212421E+04-3.92850422E+01 3.54421412E+00 3.91670541E-02
1.28715240E-06    3
-2.80329998E-08 1.30705117E-11-1.38607516E+04 1.32346197E+01
4

!Primary Thermo Library: MRH (Species ID: C4H7OJ[79])
C4H7OJ(79)              C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.11050937E+01 1.89071073E-02-6.56904732E-06 1.04000571E-09-
6.15731378E-14    2
 2.15642799E+03-3.15756194E+01 3.49728300E+00 1.99059134E-02
3.65224217E-05    3
-5.77103068E-08 2.22062786E-11 5.13502043E+03 1.24492092E+01
4

tSPC(110)               C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.17597652E+01 1.61131350E-02-5.54937997E-06 8.70882735E-10-
5.12120298E-14    2
 8.02104077E+03-3.54055376E+01 3.40986632E+00 2.51291057E-02
1.78677762E-05    3
-3.96135701E-08 1.63500158E-11 1.08981032E+04 1.09434822E+01
4
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C4H6O(105)              C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.25359380E+01 1.58064633E-02-5.17046892E-06 7.74773767E-10-
4.38510100E-14    2
-7.12479119E+03-4.40482078E+01 3.15234940E+00 2.07767775E-03
9.30849829E-05    3
-1.17019245E-07 4.26070966E-11-2.71031189E+03 1.39743214E+01
4


!!! New species with ReservoirState t-butanol oxidation chemistry
C4H6O(167)              C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.25524846E+01 1.50702522E-02-5.73038233E-06 9.68340483E-10-
5.99425090E-14    2
-1.91717129E+04-4.06801645E+01 3.69560736E+00 2.19178101E-02
2.72966753E-05    3
-5.02030764E-08 2.00937396E-11-1.59855160E+04 9.15860771E+00
4
SPC(875)                C   3H   4O   2     G   300.000  5000.000
995.043    1
 9.93166844E+00 1.36027849E-02-6.04712037E-06 1.11397211E-09-
7.25864343E-14    2
-3.67625332E+04-2.38998745E+01 4.32708078E+00 1.27451586E-02
3.05019963E-05    3
-4.69947702E-08 1.79492561E-11-3.44893542E+04 8.92910029E+00
4
SPC(194)                C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.38268844E+01 1.14068027E-02-4.28590416E-06 7.17510657E-10-
4.41022404E-14    2
-1.37390194E+03-4.81237815E+01 3.49060925E+00 2.07861875E-02
3.00728835E-05    3
-5.47955087E-08 2.20670238E-11 2.27578124E+03 9.69445748E+00
4
SPC(1454)               C   8H  10O   2     G   300.000  5000.000
995.043    1
 2.60123302E+01 2.57058444E-02-1.00577626E-05 1.73074371E-09-
1.08374228E-13    2
-3.30234083E+04-1.04709118E+02 3.12653918E+00 6.41573675E-02
1.26993173E-05    3
-6.75987969E-08 3.08983610E-11-2.58180340E+04 1.89084256E+01
4
SPC(913)                C   3H   3O   2     G   300.000  5000.000
995.043    1
 9.86948575E+00 1.10172384E-02-4.81033712E-06 8.79326931E-10-
5.70888175E-14    2
-1.47284250E+04-2.30903143E+01 4.15640831E+00 2.17221905E-02-
2.46432665E-06    3
-1.30761508E-08 6.56050523E-12-1.29844765E+04 7.49369657E+00
4
SPC(1787)               C   1H   1O   3     G   300.000  5000.000
995.043    1
 1.10893555E+01-2.12501485E-04-7.07381414E-08 3.35961525E-11-
2.98065548E-15    2
-1.62957663E+04-2.79325517E+01 3.62511537E+00 1.81643563E-02-
1.02431804E-05    3
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-4.89599442E-09 4.18643591E-12-1.42346267E+04 1.09337985E+01
4


C5H10_iso         T11/95C   5H  10    0    0G   298.150  5000.000 1000.
1
 0.10169614E+02 0.29142736E-01-0.11304015E-04 0.20426202E-08-
0.13964602E-12    2
-0.97185802E+04-0.27826511E+02 0.15343285E+01 0.40535723E-01
0.26841152E-05    3
-0.27784359E-07 0.12941501E-10-0.66019829E+04 0.20108917E+02-
0.43679207E+04    4
C5H9J(5)               C   5H   9          G   300.000  5000.000
995.043    1
 1.18048007E+01 2.30859604E-02-8.00000750E-06 1.26443258E-09-
7.47975462E-14    2
 1.99192609E+04-3.46915777E+01 3.44256134E+00 2.78474243E-02
2.83190385E-05    3
-5.22112380E-08 2.06826060E-11 2.30118566E+04 1.27876110E+01
4
C5H9J(7)               C   5H   9          G   300.000  5000.000
995.043    1
 1.28725898E+01 2.22396319E-02-7.55953546E-06 1.17527023E-09-
6.86363774E-14    2
 7.79518845E+03-4.27413861E+01 3.26218009E+00 2.34770461E-02
4.69481570E-05    3
-7.31134978E-08 2.80854394E-11 1.15590372E+04 1.28781159E+01
4
C5H9J(8)               C   5H   9          G   300.000  5000.000
995.043    1
 1.15808333E+01 2.38320359E-02-8.32367016E-06 1.32079890E-09-
7.83149172E-14    2
 6.77970002E+03-3.58988147E+01 3.47279923E+00 2.58394377E-02
3.47582568E-05    3
-5.84353977E-08 2.26965907E-11 9.90745887E+03 1.07861409E+01
4
C5H9J(9)               C   5H   9          G   300.000  5000.000
995.043    1
 1.13430909E+01 2.36131612E-02-8.23696637E-06 1.30793336E-09-
7.76209514E-14    2
 1.49508237E+04-3.11892183E+01 3.50164434E+00 2.55322728E-02
3.34956486E-05    3
-5.65510456E-08 2.19710816E-11 1.79768470E+04 1.39663072E+01
4
C5H11J(10)             C   5H  11          G   300.000  5000.000
995.043    1
 8.86924469E+00 3.17129517E-02-1.14345618E-05 1.85720895E-09-
1.11990315E-13    2
-7.94927900E+02-1.80248382E+01 3.87955200E+00 2.95797299E-02
2.52341843E-05    3
-4.51234970E-08 1.73228868E-11 1.29666140E+03 1.15431026E+01
4
C5H11J(11)             C   5H  11          G   300.000  5000.000
995.043    1
 1.13005282E+01 2.85671921E-02-9.52656141E-06 1.45792525E-09-
8.41744102E-14    2
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 5.32727050E+02-3.20023937E+01 3.23582221E+00 2.79925382E-02
4.10775584E-05    3
-6.57699814E-08 2.51789764E-11 3.77106658E+03 1.50727305E+01
4

!New thermo from C5H10_iso RMG run
C5H8(95)                C   5H   8          G   300.000  5000.000
995.043    1
 1.33033492E+01 1.85576639E-02-6.01408510E-06 9.03112111E-10-
5.14041996E-14    2
 3.04021248E+03-4.61967623E+01 3.11506942E+00 2.41456110E-02
3.88788393E-05    3
-6.48960876E-08 2.54552080E-11 6.81868801E+03 1.17033851E+01
4

SPC(482)                C   8H  13          G   300.000  5000.000
995.043    1
 2.03145343E+01 3.33517778E-02-1.18843961E-05 1.91698200E-09-
1.15011349E-13    2
 2.33739727E+04-7.69200762E+01 3.02149829E+00 5.25550335E-02
3.50134510E-05    3
-8.03200729E-08 3.33139830E-11 2.93062301E+04 1.89389084E+01
4

SPC(483)                C   8H  13          G   300.000  5000.000
995.043    1
 1.54190427E+01 3.89587529E-02-1.41730970E-05 2.31692245E-09-
1.40328919E-13    2
 2.39229318E+04-4.61292270E+01 3.54706920E+00 5.60806813E-02
6.14856880E-06    3
-4.22065733E-08 1.88115498E-11 2.78005506E+04 1.86998946E+01
4

C5H7J(504)              C   5H   7          G   300.000  5000.000
995.043    1
 1.11544424E+01 1.89877286E-02-6.64387894E-06 1.05733068E-09-
6.28392066E-14    2
 3.67400140E+04-2.94061316E+01 3.52149603E+00 2.28026596E-02
2.81094465E-05    3
-4.93643246E-08 1.94235093E-11 3.95891972E+04 1.40644316E+01
4

SPC(493)                C   8H  11          G   300.000  5000.000
995.043    1
 1.95448740E+01 2.92191209E-02-1.05030196E-05 1.70521023E-09-
1.02769853E-13    2
 3.86194166E+04-7.20294322E+01 3.11070106E+00 4.99837092E-02
2.64828426E-05    3
-6.88269521E-08 2.91131205E-11 4.41325372E+04 1.84430416E+01
4

SPC(494)                C   8H  11          G   300.000  5000.000
995.043    1
 1.66650676E+01 3.23060953E-02-1.11819303E-05 1.76286096E-09-
1.04099582E-13    2
 3.94339624E+04-5.46516974E+01 3.07594673E+00 6.11153283E-02-
1.56910573E-05    3
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-2.12920161E-08 1.22397956E-11 4.34164494E+04 1.72629400E+01
4

SPC(495)               C   8H  11          G   300.000  5000.000
995.043    1
 1.87492399E+01 3.01404060E-02-1.05674959E-05 1.68270512E-09-
1.00025742E-13    2
 3.14399011E+04-6.81039434E+01 3.00281508E+00 4.97888662E-02
2.56157251E-05    3
-6.66466606E-08 2.81440890E-11 3.67345406E+04 1.86438616E+01
4

SPC(496)               C   8H  11          G   300.000  5000.000
995.043    1
 1.70746426E+01 3.21521189E-02-1.12048005E-05 1.77299768E-09-
1.04876979E-13    2
 3.15403088E+04-6.00935196E+01 3.05655099E+00 4.27203077E-02
4.18813648E-05    3
-8.00349348E-08 3.20667987E-11 3.65965656E+04 1.88551473E+01
4

SPC(498)               C   7H  11          G   300.000  5000.000
995.043    1
 1.30694421E+01 3.34190422E-02-1.21543907E-05 1.98642382E-09-
1.20291475E-13    2
 2.71471329E+04-3.60959567E+01 3.65961481E+00 4.57515327E-02
7.68673259E-06    3
-3.70558785E-08 1.61582276E-11 3.02818790E+04 1.55962466E+01
4

SPC(499)               C   7H  11          G   300.000  5000.000
995.043    1
 1.79649338E+01 2.78120671E-02-9.86568977E-06 1.58648337E-09-
9.49739051E-14    2
 2.65981739E+04-6.61937284E+01 3.13404390E+00 4.22258849E-02
3.65516148E-05    3
-7.51693782E-08 3.06606607E-11 3.17875585E+04 1.65283378E+01
4

C6H7J(511)             C   6H   7          G   300.000  5000.000
995.043    1
 1.66640544E+01 1.59343681E-02-5.03611781E-06 7.38345612E-10-
4.11838334E-14    2
 3.73402776E+04-6.29156778E+01 2.82351279E+00 3.39071899E-02
2.46495398E-05    3
-5.71920661E-08 2.40712947E-11 4.19592964E+04 1.31577639E+01
4

C6H7J(512)             C   6H   7          G   300.000  5000.000
995.043    1
 1.28544144E+01 2.00759075E-02-7.07067192E-06 1.13138031E-09-
6.75139112E-14    2
 5.29407756E+04-3.64685169E+01 3.43715773E+00 3.08555568E-02
1.74972048E-05    3
-4.26763058E-08 1.78099062E-11 5.61553529E+04 1.56532071E+01
4
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C6H7J(505)              C   6H   7          G   300.000  5000.000
995.043    1
 1.55962653E+01 1.67806966E-02-5.47658986E-06 8.27507961E-10-
4.73450021E-14    2
 4.94643501E+04-5.48658695E+01 3.00389404E+00 3.82775681E-02
6.02042129E-06    3
-3.62898062E-08 1.66684613E-11 5.34121158E+04 1.30672590E+01
4

C6H7J(506)              C   6H   7          G   300.000  5000.000
995.043    1
 1.39528205E+01 1.86518652E-02-6.33695224E-06 9.87924773E-10-
5.78745890E-14    2
 4.90227736E+04-4.48120383E+01 3.23393085E+00 3.53985152E-02
8.12854802E-06    3
-3.53094234E-08 1.57462162E-11 5.24600237E+04 1.34001213E+01
4


!New species from C8H14 RMG run
C8H13J(41)              C   8H  13          G   300.000  5000.000
995.043    1
 1.89378884E+01 3.47658385E-02-1.21605833E-05 1.93330779E-09-
1.14807487E-13    2
 9.65071081E+03-6.98870301E+01 2.98296340E+00 5.25184794E-02
3.10019272E-05    3
-7.38333815E-08 3.06916613E-11 1.51221905E+04 1.85457372E+01
4

C8H15J(44)              C   8H  15          G   300.000  5000.000
995.043    1
 1.56076912E+01 4.35841855E-02-1.57661844E-05 2.56752513E-09-
1.55110664E-13    2
 2.13374148E+03-4.86053912E+01 3.52721752E+00 5.88102946E-02
1.15347709E-05    3
-4.93932942E-08 2.13591221E-11 6.18820046E+03 1.79086928E+01
4

SPC(425)                C  11H  17          G   300.000  5000.000
995.043    1
 2.70529808E+01 4.52230116E-02-1.62160187E-05 2.62729817E-09-
1.58131698E-13    2
 2.63026421E+04-1.07500629E+02 2.66916381E+00 8.17855982E-02
2.13140376E-05    3
-8.45898702E-08 3.73502184E-11 3.41977691E+04 2.53044985E+01
4

SPC(426)                C  11H  17          G   300.000  5000.000
995.043    1
 2.21574892E+01 5.08299868E-02-1.85047196E-05 3.02723863E-09-
1.83449268E-13    2
 2.68516012E+04-7.67097800E+01 3.19473472E+00 8.53112460E-02-
7.55084464E-06    3
-4.64763705E-08 2.28477852E-11 3.26920897E+04 2.50654847E+01
4
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C7H10(454)              C   7H  10          G   300.000  5000.000
995.043    1
 1.49671204E+01 2.82320366E-02-9.44959426E-06 1.44992821E-09-
8.38814476E-14    2
 1.90191571E+04-4.86918216E+01 3.00020853E+00 4.56574388E-02
1.05324352E-05    3
-4.29249680E-08 1.88504989E-11 2.29195394E+04 1.66142973E+01
4


!8APR2010
CH3CHCHCHO              C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.17479322E+01 1.60438314E-02-6.18293985E-06 1.05276871E-09-
6.54738507E-14    2
-1.93853246E+04-3.56538534E+01 3.80989515E+00 1.85437310E-02
3.43839630E-05    3
-5.58307733E-08 2.16893064E-11-1.63496088E+04 9.91929863E+00
4

CHCHCHO                 C   3H   3O   1     G   300.000  5000.000
995.043    1
 1.03627471E+01 6.83571269E-03-2.78010453E-06 4.90649245E-10-
3.11934576E-14    2
 1.53576845E+04-2.82037694E+01 3.79724059E+00 1.15701693E-02
2.27322885E-05    3
-3.84770898E-08 1.52552052E-11 1.77364868E+04 8.82613673E+00
4

CH3CCHCHO               C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.09942563E+01 1.43724675E-02-5.70006523E-06 9.87732057E-10-
6.21246916E-14    2
 9.80529905E+03-2.93643218E+01 3.92086719E+00 2.23139310E-02
1.32211095E-05    3
-3.23869740E-08 1.35233347E-11 1.22274828E+04 9.82340524E+00
4

!Primary Thermo Library: MRH (Species ID: CH3CHCHCO)
CH3CHCHCO               C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.09774324E+01 1.37178553E-02-4.71706433E-06 7.41678192E-10-
4.37120337E-14    2
 2.47750140E+03-3.04181661E+01 3.48792583E+00 2.45706428E-02
7.94826975E-06    3
-2.71907565E-08 1.18601099E-11 4.92118041E+03 1.04669137E+01
4

C4H7O-14                C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.27295312E+01 1.65976440E-02-6.61510112E-06 1.15513075E-09-
7.30598341E-14    2
-1.77392598E+03-3.67162035E+01 3.92516155E+00 2.46633563E-02
2.24210945E-05    3
-4.58989494E-08 1.86834853E-11 1.33106662E+03 1.25139744E+01
4
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!Burcat 30-SEPT-2010
C12H10 biphenyl   g 8/00C 12.H 10.   0.   0.G   200.000  6000.000 1000.
1
 2.28963620E+01 3.68453189E-02-1.35016357E-05 2.20802787E-09-
1.33358137E-13    2
 1.07395923E+04-1.00509573E+02 1.94600056E-01 5.35259888E-02
8.55000841E-05    3
-1.63903525E-07 7.29975666E-11 1.90021492E+04 2.72148992E+01
2.19050792E+04    4

!10Jul2010
!RMG estimate
biC5H5                  C  10H  10          G   300.000  5000.000
995.043    1
 2.42357727E+01 2.88285511E-02-9.88027549E-06 1.54550884E-09-
9.06124695E-14    2
 2.19801813E+04-1.24312702E+02 2.46682055E+00 4.98067248E-02
5.87900370E-05    3
-1.11658772E-07 4.52341424E-11 2.96060617E+04-2.84786672E+00
4
!Primary Thermo Library: MRH (Species ID: C5H4C5H5)
C5H4C5H5                C  10H   9          G   250.000  5000.000
995.043    1
 2.29745100E+01 2.65226742E-02-8.92155605E-06 1.37686293E-09-
7.98953825E-14    2
 4.00055111E+04-9.78749035E+01 2.47330528E+00 3.28096056E-02
9.63595924E-05    3
-1.46047067E-07 5.62771691E-11 4.78541037E+04 1.98669401E+01
4
!Primary Thermo Library: MRH (Species ID: fulvalene)
fulvalene               C  10H   8          G   250.000  5000.000
995.043    1
 2.21715504E+01 2.48738071E-02-8.31664351E-06 1.27753861E-09-
7.38517298E-14    2
 3.53794187E+04-9.71735123E+01 2.51070252E+00 2.54744285E-02
1.09015916E-04    3
-1.56551883E-07 5.94832468E-11 4.31750385E+04 1.70924452E+01
4
!RMG estimate
!C10H8                   C  10H   8          G   300.000  5000.000
995.043    1
! 2.69189602E+01 2.15713834E-02-6.55235633E-06 9.17630326E-10-
4.90147707E-14    2
! 2.64510808E+04-1.57796580E+02 1.76738172E+00 4.47088189E-02
7.61063843E-05    3
!-1.33211637E-07 5.34356643E-11 3.53164089E+04-1.71838511E+01
4
!Active Thermochemical Tables (17-DEC-2010)
C10H8 Naphthalene T 7/98C  10H   8    0    0G   200.000  6000.000 1000.
1
 1.86129884E+01 3.04494175E-02-1.11224825E-05 1.81615474E-09-
1.09601281E-13    2
 8.91578988E+03-8.00230396E+01-1.04919475E+00 4.62970781E-02
7.07591636E-05    3
-1.38408111E-07 6.20475407E-11 1.59848987E+04 3.02121626E+01
1.81107678E+04    4
!RMG estimate
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!C10H9                    C  10H   9          G   300.000  5000.000
995.043    1
! 2.50288494E+01 2.58118605E-02-8.02693596E-06 1.15108671E-09-
6.28380917E-14    2
! 3.08581976E+04-1.28597031E+02 1.89792700E+00 3.64615840E-02
1.00036541E-04    3
!-1.54407467E-07 5.99134478E-11 3.95374805E+04 3.36303786E+00
4
!Active Thermochemical Tables (17-DEC-2010)
C10H9 2-hydro Rad T 7/98C  10H   9    0    0G   200.000  6000.000 1000.
1
 1.96879334E+01 3.20520257E-02-1.16715110E-05 1.90182471E-09-
1.14603906E-13    2
 1.80099777E+04-8.29833882E+01-1.21356342E+00 5.48913745E-02
5.55281159E-05    3
-1.24860759E-07 5.75105005E-11 2.52575495E+04 3.28077928E+01
2.76064663E+04    4

iBuOH                     C   4H  10O   1     G   300.000  5000.000
995.043    1
 1.28027466E+01 2.40684085E-02-9.15947102E-06 1.56143608E-09-
9.73970454E-14    2
-4.04757328E+04-4.08733835E+01 3.43413365E+00 2.42080917E-02
4.71925488E-05    3
-7.40899903E-08 2.84309440E-11-3.67537796E+04 1.36120661E+01
4
C4H9Oi1                   C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.18522891E+01 2.24318167E-02-8.23872040E-06 1.37180064E-09-
8.42985697E-14    2
-1.52255287E+04-3.25751767E+01 3.28769309E+00 2.76289432E-02
2.79930939E-05    3
-5.24269958E-08 2.08501567E-11-1.20739593E+04 1.59732410E+01
4
C4H9Oi3                   C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.33486992E+01 2.08631055E-02-7.99230949E-06 1.37115111E-09-
8.59204677E-14    2
-1.85371039E+04-4.21989889E+01 3.37615919E+00 3.12478786E-02
2.11310768E-05    3
-4.81419874E-08 1.98916024E-11-1.50819657E+04 1.32524097E+01
4
C4H9Oi2                   C   4H   9O   1     G   300.000  5000.000
995.043    1
 9.42100551E+00 2.55775763E-02-1.01467208E-05 1.77108434E-09-
1.12114475E-13    2
-1.65531837E+04-1.85976213E+01 3.93142288E+00 2.92161348E-02
1.21497198E-05    3
-3.17805114E-08 1.29940670E-11-1.45483645E+04 1.24436132E+01
4
C4H9Oi4                   C   4H   9O   1     G   300.000  5000.000
995.043    1
 1.27002231E+01 2.23129950E-02-8.64097052E-06 1.48678467E-09-
9.32398384E-14    2
-1.42014723E+04-4.04698462E+01 3.46392887E+00 2.26205697E-02
4.64030229E-05    3
```

```
-7.25814864E-08 2.78597619E-11-1.05404958E+04 1.32038158E+01
4
C4H8O-i3                C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.20954055E+01 2.06992084E-02-8.40015737E-06 1.48596599E-09-
9.47605236E-14    2
-3.14349479E+04-3.74889362E+01 3.68165222E+00 1.88948172E-02
4.80267563E-05    3
-7.23023233E-08 2.74847639E-11-2.79968028E+04 1.19233619E+01
4

C4H8O-i2                C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.19559389E+01 1.98568964E-02-6.79050433E-06 1.07334472E-09-
6.36480247E-14    2
-2.84607944E+04-3.62316210E+01 2.93882215E+00 3.10486818E-02
1.41099834E-05    3
-3.82363813E-08 1.61709247E-11-2.54258827E+04 1.34589842E+01
4
C4H8O-i1                C   4H   8O   1     G   300.000  5000.000
995.043    1
 1.03650689E+01 2.19479713E-02-7.86865946E-06 1.28459092E-09-
7.78785264E-14    2
-2.40496722E+04-2.58754104E+01 3.24243011E+00 2.92434559E-02
1.32985566E-05    3
-3.44473251E-08 1.43139782E-11-2.15759067E+04 1.37596173E+01
4

!21Jul2010 : Iso-butanol chemistry
!Estimated by RMG using Group Additivity
iC4H7OJ(15)             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.32231978E+01 1.62811919E-02-5.40963908E-06 8.27419337E-10-
4.77486385E-14    2
-1.06869559E+04-4.37059364E+01 3.21064973E+00 2.65706362E-02
2.42436043E-05    3
-4.92994339E-08 2.01489687E-11-7.21117458E+03 1.20020011E+01
4

!Estimated by RMG using Group Additivity
iC4H7OJ(17)             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.16323278E+01 1.83722669E-02-6.48779421E-06 1.03866554E-09-
6.19791403E-14    2
-6.27583363E+03-3.33497258E+01 3.51425769E+00 2.47654104E-02
2.34321775E-05    3
-4.55103777E-08 1.82920222E-11-3.36119861E+03 1.23026342E+01
4

!Estimated by RMG using Group Additivity
iC4H7OJ(30)             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.04853654E+01 1.97765845E-02-6.99385815E-06 1.12171256E-09-
6.70522985E-14    2
-9.77677020E+03-2.79619206E+01 3.61486443E+00 2.62607283E-02
1.50915680E-05    3
```

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-3.50211377E-08 1.43767316E-11-7.36319409E+03 1.04076324E+01
4

!Estimated by RMG using Group Additivity
iC4H7OJ(48)             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.11378070E+01 1.91503616E-02-7.54301969E-06 1.30123499E-09-
8.16029303E-14    2
-6.20871619E+03-2.92214278E+01 4.01203735E+00 1.89692457E-02
3.61847140E-05    3
-5.71099490E-08 2.19087364E-11-3.36357170E+03 1.22917040E+01
4

!Estimated by RMG using Group Additivity
iC4H7OJ(51)             C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.17861482E+01 1.85934728E-02-7.75164709E-06 1.38376729E-09-
8.85985648E-14    2
-1.25871640E+04-3.43309918E+01 4.20682791E+00 1.61342760E-02
4.55928632E-05    3
-6.76128296E-08 2.56020092E-11-9.44872108E+03 1.03882535E+01
4

!Estimated by RMG using Group Additivity
C3H3OH                  C   3H   4O   1     G   300.000  5000.000
995.043    1
 1.01683537E+01 8.92821108E-03-2.86220065E-06 4.27194504E-10-
2.42058692E-14    2
-1.87445093E+03-2.76353401E+01 3.44746182E+00 1.47603283E-02
2.02824298E-05    3
-3.64764246E-08 1.46235600E-11 5.11857136E+02 1.00257689E+01
4

!Estimated by RMG using Group Additivity
C4H6Oi-12               C   4H   6O   1     G   300.000  5000.000
995.043    1
 9.56306281E+00 1.77749855E-02-6.22150416E-06 9.90762511E-10-
5.89329791E-14    2
-1.52696984E+04-2.33978868E+01 3.63921276E+00 2.20905564E-02
1.66654119E-05    3
-3.40358309E-08 1.36890260E-11-1.31255492E+04 1.00021322E+01
4

!Primary Thermo Library: MRH (Species ID: C4H6Oi-13)
C4H6Oi-13               C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.09035339E+01 1.71664263E-02-6.17336779E-06 9.99573390E-10-
6.00733902E-14    2
-1.77348201E+04-3.16143061E+01 3.60619688E+00 1.56689529E-02
4.25627989E-05    3
-6.27932839E-08 2.37914314E-11-1.47562219E+04 1.12247118E+01
4

!Primary Thermo Library: MRH (Species ID: iC4H5OJ(14))
iC4H5OJ(14)             C   4H   5O   1     G   300.000  5000.000
995.043    1
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```
 1.10521695E+01 1.30492089E-02-4.22892685E-06 6.35786751E-10-
3.62567157E-14    2
 2.53601205E+03-2.97689300E+01 3.35333469E+00 2.67344148E-02
1.16533442E-06    3
-2.04142961E-08 9.63319583E-12 4.92278699E+03 1.16297313E+01
4

!Estimated by RMG using Group Additivity
iC4H5OJ(15)             C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.38268844E+01 1.14068027E-02-4.28590416E-06 7.17510657E-10-
4.41022404E-14    2
-1.37390194E+03-4.81237815E+01 3.49060925E+00 2.07861875E-02
3.00728835E-05    3
-5.47955087E-08 2.20670238E-11 2.27578124E+03 9.69445748E+00
4

!Estimated by RMG using Group Additivity
C3H3OJ(9)               C   3H   3O   1     G   300.000  5000.000
995.043    1
 9.59142550E+00 6.89889691E-03-1.73752751E-06 1.97077588E-10-
8.35408900E-15    2
 1.71360208E+04-2.27072529E+01 3.23401046E+00 1.80183918E-02
3.26330095E-06    3
-1.77344757E-08 8.16029266E-12 1.91159045E+04 1.15233280E+01
4

!Estimated by RMG using Group Additivity
HCCCHO                  C   3H   2O   1     G   300.000  5000.000
995.043    1
 8.23328705E+00 6.91012199E-03-2.59686617E-06 4.32413940E-10-
2.64777283E-14    2
 8.69264315E+03-1.74534515E+01 3.79681359E+00 1.38711784E-02
3.30065358E-06    3
-1.45007084E-08 6.48454322E-12 1.01138249E+04 6.63275736E+00
4

!Estimated by RMG using Group Additivity
C3H3OJ                  C   3H   3O   1     G   300.000  5000.000
995.043    1
 6.23461636E+00 1.10890491E-02-4.02000033E-06 6.55742026E-10-
3.96704443E-14    2
 1.85380822E+04-3.90352835E+00 3.93746524E+00 1.50247660E-02-
1.96539361E-06    3
-6.07241080E-09 2.99531061E-12 1.92575480E+04 8.48558161E+00
4

!Estimated by RMG using Group Additivity
C3H5OJ                  C   3H   5O   1     G   300.000  5000.000
995.043    1
 7.32929813E+00 1.46987662E-02-5.38979945E-06 8.87792713E-10-
5.40686027E-14    2
 1.04039152E+04-8.55819199E+00 3.93663805E+00 1.60444184E-02
1.11124215E-05    3
-2.25838789E-08 8.96239152E-12 1.16876348E+04 1.08504865E+01
4
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!Estimated by RMG using Group Additivity
C3H5OJ(17)              C   3H   5O   1     G   300.000  5000.000
995.043    1
 8.92016807E+00 1.26076912E-02-4.31164432E-06 6.76546514E-10-
3.98381009E-14    2
 5.99279294E+03-1.89144026E+01 3.63303008E+00 1.78496442E-02
1.19238483E-05    3
-2.63729351E-08 1.08193380E-11 7.83765879E+03 1.05498534E+01
4

!ATcT (12/Aug/2010)
nC3H7OH           g 2/00C  3.H  8.O  1.   0.G   200.000  6000.000 1000.
1
 8.52377408E+00 2.10371210E-02-7.48398370E-06 1.19958663E-09-
7.14873013E-14    2
-3.50702414E+04-1.77857176E+01 5.41877541E+00-5.75566129E-04
8.51215375E-05    3
-1.11060442E-07 4.43007063E-11-3.28368377E+04 5.29974117E+00-
3.06933301E+04    4

!Estimated by RMG using Group Additivity
C4H7OJ(9)               C   4H   7O   1     G   300.000  5000.000
995.043    1
 1.23022972E+01 1.67877287E-02-5.66216616E-06 8.78339775E-10-
5.12543188E-14    2
-2.05002171E+03-3.47818474E+01 3.33394275E+00 2.28529739E-02
3.03990660E-05    3
-5.35686708E-08 2.12376370E-11 1.21927378E+03 1.59002697E+01
4

!Estimated by RMG using Group Additivity
C4H9O2J(52)             C   4H   9O   2     G   300.000  5000.000
995.043    1
 1.38239911E+01 2.34837071E-02-1.04711179E-05 1.94318728E-09-
1.27319596E-13    2
-3.41585451E+04-3.71806954E+01 4.71174228E+00 2.79408037E-02
3.13105855E-05    3
-5.85449050E-08 2.32342255E-11-3.07523650E+04 1.47388527E+01
4

!Estimated by RMG using Group Additivity
C4H9O2J(53)             C   4H   9O   2     G   300.000  5000.000
995.043    1
 1.49762960E+01 2.16117873E-02-8.34318886E-06 1.42698017E-09-
8.90865993E-14    2
-3.53980340E+04-4.50327333E+01 3.75933303E+00 3.35669046E-02
2.35868131E-05    3
-5.34329855E-08 2.21027269E-11-3.15253349E+04 1.72698855E+01
4

C4H9O2J(54)             C   4H   9O   2     G   300.000  5000.000
995.043    1
 1.37757565E+01 2.31432421E-02-9.19585566E-06 1.59958967E-09-
1.00907879E-13    2
-3.63314411E+04-3.78496393E+01 4.02309249E+00 3.12722721E-02
2.53960400E-05    3
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-5.29629447E-08 2.14933687E-11-3.28521457E+04 1.68833415E+01
4

C4H9O2J(55)             C   4H   9O   2     G   300.000  5000.000
995.043    1
 1.37757565E+01 2.31432421E-02-9.19585566E-06 1.59958967E-09-
1.00907879E-13    2
-3.63314411E+04-3.78496393E+01 4.02309249E+00 3.12722721E-02
2.53960400E-05    3
-5.29629447E-08 2.14933687E-11-3.28521457E+04 1.68833415E+01
4

!Estimated by RMG using Group Additivity
CH2CHCHCHOH             C   4H   6O   1     G   300.000  5000.000
995.043    1
 1.42625555E+01 1.17322315E-02-3.43928489E-06 4.73518531E-10-
2.50375670E-14    2
-1.41367601E+04-4.96333931E+01 2.94736783E+00 2.14663121E-02
3.57822568E-05    3
-6.19137128E-08 2.47217635E-11-1.01150124E+04 1.37933460E+01
4

!Estimated by RMG using Group Additivity
CH2CHCCHOH              C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.28765838E+01 1.13931952E-02-3.23658958E-06 4.26643239E-10-
2.16067239E-14    2
 1.06641991E+04-4.04279819E+01 2.96386521E+00 2.78508763E-02
7.21479441E-06    3
-3.02000306E-08 1.36087234E-11 1.37948849E+04 1.31645877E+01
4

!Estimated by RMG using Group Additivity
CHCHCHCHOH              C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.44691661E+01 8.91511046E-03-2.43527876E-06 3.11851055E-10-
1.53584672E-14    2
 1.57851233E+04-4.90272017E+01 2.92275097E+00 2.47050678E-02
1.99293465E-05    3
-4.56038853E-08 1.92922143E-11 1.95991043E+04 1.42386908E+01
4

!Estimated by RMG using Group Additivity
CH2CHCHCOH              C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.44691661E+01 8.91511046E-03-2.43527876E-06 3.11851055E-10-
1.53584672E-14    2
 1.57851233E+04-4.90272017E+01 2.92275097E+00 2.47050678E-02
1.99293465E-05    3
-4.56038853E-08 1.92922143E-11 1.95991043E+04 1.42386908E+01
4

!Estimated by RMG using Group Additivity
CHCCHCHOH               C   4H   4O   1     G   300.000  5000.000
995.043    1
 1.34958165E+01 8.38681784E-03-2.66137975E-06 3.92427953E-10-
2.19786180E-14    2
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 7.63576028E+03-4.52261294E+01 3.19144714E+00 2.12169751E-02
2.11001690E-05    3
-4.44057879E-08 1.84889040E-11 1.11019122E+04 1.15480187E+01
4

!Estimated by RMG using Group Additivity
CHCCCHOH                C   4H   3O   1     G   300.000  5000.000
995.043    1
 1.16777310E+01 7.93905058E-03-2.20403840E-06 2.83140914E-10-
1.39739914E-14    2
 3.36382749E+04-3.19825514E+01 3.14745194E+00 2.89115933E-02-
1.37422068E-05    3
-5.43802185E-09 4.80309511E-12 3.59952156E+04 1.24418569E+01
4

!Estimated by RMG using Group Additivity
C4H5O3J(1)              C   4H   5O   3     G   300.000  5000.000
995.043    1
 1.48579085E+01 1.51500789E-02-5.25421053E-06 8.31315852E-10-
4.92025399E-14    2
-1.75361472E+04-4.39114794E+01 3.23618755E+00 3.60955349E-02
2.02321369E-06    3
-3.00749301E-08 1.42558873E-11-1.39474188E+04 1.85101660E+01
4

!Estimated by RMG using Group Additivity
C4H5O3J(2)              C   4H   5O   3     G   300.000  5000.000
995.043    1
 1.61490627E+01 1.43429309E-02-5.26812589E-06 8.66498285E-10-
5.26595192E-14    2
-1.25208354E+04-5.02485159E+01 3.29721039E+00 4.16168356E-02-
9.61611845E-06    3
-2.08536308E-08 1.15934129E-11-8.75578671E+03 1.77575515E+01
4

!Estimated by RMG using Group Additivity
OCOOH                   C   1H   1O   3     G   300.000  5000.000
995.043    1
 1.10893555E+01-2.12501485E-04-7.07381414E-08 3.35961525E-11-
2.98065548E-15    2
-1.62957663E+04-2.79325517E+01 3.62511537E+00 1.81643563E-02-
1.02431804E-05    3
-4.89599442E-09 4.18643591E-12-1.42346267E+04 1.09337985E+01
4

!Estimated by RMG using Group Additivity
C4H6O3(21)              C   4H   6O   3     G   300.000  5000.000
995.043    1
 1.69027387E+01 1.60142949E-02-5.75100051E-06 9.31534933E-10-
5.60086783E-14    2
-4.17114590E+04-5.65380475E+01 3.18623835E+00 3.78466355E-02
1.15467351E-05    3
-4.42974301E-08 1.97593846E-11-3.73328783E+04 1.78534449E+01
4

!Estimated by RMG using Group Additivity
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```
C4H5O2J(12)             C   4H   5O   2     G   300.000  5000.000
995.043    1
 1.29859292E+01 1.47264189E-02-5.87873217E-06 1.02481710E-09-
6.46974945E-14    2
-2.34752735E+04-3.91025330E+01 3.82644729E+00 2.16793824E-02
2.86642967E-05    3
-5.22844231E-08 2.09080359E-11-2.01738530E+04 1.24710117E+01
4

!Estimated by RMG using Group Additivity
CH2CHCHCHO              C   4H   5O   1     G   300.000  5000.000
995.043    1
 1.30223320E+01 1.23803820E-02-4.73846167E-06 8.01938880E-10-
4.96335821E-14    2
-1.58751364E+03-4.30974704E+01 3.60489704E+00 1.74121083E-02
3.71601712E-05    3
-6.04232057E-08 2.36625907E-11 1.91168846E+03 1.04551484E+01
4

!Estimated by RMG using Group Additivity
C4H5O2J(13)             C   4H   5O   2     G   300.000  5000.000
995.043    1
 1.39147448E+01 1.42983435E-02-6.13015122E-06 1.11234709E-09-
7.19027144E-14    2
-8.99174257E+03-4.22037782E+01 3.98962009E+00 2.31976046E-02
2.71846399E-05    3
-5.25168226E-08 2.12683433E-11-5.48193552E+03 1.33412264E+01
4

!Estimated by RMG using Group Additivity
C4H6O3(3)               C   4H   6O   3     G   300.000  5000.000
995.043    1
 1.68938386E+01 1.68988238E-02-7.07692140E-06 1.26382439E-09-
8.09025220E-14    2
-2.81040398E+04-5.58076339E+01 3.77817983E+00 3.80737326E-02
8.56187654E-06    3
-4.10782055E-08 1.85630833E-11-2.39320578E+04 1.52508328E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(1)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.51195526E+01 1.97839073E-02-6.90967497E-06 1.09928731E-09-
6.53514361E-14    2
-3.08678452E+04-4.66537490E+01 3.25158795E+00 4.36396109E-02-
6.91426951E-06    3
-2.29885462E-08 1.20393405E-11-2.73251809E+04 1.64769447E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(2)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.43672164E+01 2.14461729E-02-7.84944827E-06 1.28635981E-09-
7.80068959E-14    2
-3.05033424E+04-4.00107194E+01 3.47344490E+00 4.57039285E-02-
1.49697518E-05    3
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-1.36726633E-08 8.63733792E-12-2.73683274E+04 1.73506893E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(3)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.71013127E+01 1.73347769E-02-5.85414439E-06 9.09562228E-10-
5.31482737E-14    2
-2.17564965E+04-5.66424107E+01 3.00537291E+00 4.22715628E-02
4.38323432E-06    3
-3.79941494E-08 1.77723424E-11-1.73805795E+04 1.91849476E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(4)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.76827103E+01 1.80309359E-02-6.49067525E-06 1.05324471E-09-
6.34178033E-14    2
-2.21261870E+04-6.09685800E+01 3.15464030E+00 4.25811329E-02
7.53092759E-06    3
-4.25307856E-08 1.94768868E-11-1.75591365E+04 1.74697075E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(5)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.67274950E+01 1.80600749E-02-7.20719360E-06 1.25847147E-09-
7.95746720E-14    2
-1.84655836E+04-5.31426106E+01 3.68903230E+00 3.79657625E-02
1.17904346E-05    3
-4.43024110E-08 1.96164587E-11-1.42614935E+04 1.77823497E+01
4

!Estimated by RMG using Group Additivity
C4H7O3J(6)              C   4H   7O   3     G   300.000  5000.000
995.043    1
 1.87036796E+01 1.70955058E-02-7.14211404E-06 1.27733594E-09-
8.18646763E-14    2
-1.12785709E+04-6.55442565E+01 3.67548169E+00 3.81107562E-02
2.05679025E-05    3
-5.70785826E-08 2.45769898E-11-6.33746162E+03 1.66838574E+01
4

!Estimated by RMG using Group Additivity
C3H5O2J(54)             C   3H   5O   2     G   300.000  5000.000
995.043    1
 1.36677597E+01 1.10717126E-02-3.62566826E-06 5.46025832E-10-
3.10882009E-14    2
 5.38332949E+03-4.40256889E+01 3.17578189E+00 2.54084180E-02
1.67306138E-05    3
-4.12108112E-08 1.75247426E-11 8.84957031E+03 1.34654675E+01
4

!Estimated by RMG using Group Additivity
C4H5O3J(3)              C   4H   5O   3     G   300.000  5000.000
995.043    1
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 1.48490084E+01 1.60346079E-02-6.58013143E-06 1.16360531E-09-
7.40963836E-14    2
-9.02635271E+03-4.31810658E+01 3.82812903E+00 3.63226320E-02-
9.61644821E-07    3
-2.68557055E-08 1.30595860E-11-5.64422305E+03 1.59075540E+01
4

!Estimated by RMG using Group Additivity
CH2CHCH2O               C   3H   5O   1     G   300.000  5000.000
995.043    1
 8.01432843E+00 1.45413452E-02-5.31080453E-06 8.71474747E-10-
5.29016276E-14    2
 7.47799128E+03-1.46228014E+01 3.86206459E+00 1.06681114E-02
3.15292215E-05    3
-4.45813498E-08 1.65853970E-11 9.32240974E+03 1.05046087E+01
4

!Primary Thermo Library: Franklin (Species ID: npropoxy)
OCH2CH2CH3              C   3H   7O   1     G   300.000  5000.000
995.043    1
 8.94585327E+00 1.83434671E-02-6.43818142E-06 1.02716643E-09-
6.11730125E-14    2
-7.79454216E+03-4.45074923E+00 3.69109320E+00 1.87568520E-02
2.41589739E-05    3
-4.03897982E-08 1.56000140E-11-5.72352256E+03 2.60262430E+01
4

!Estimated by RMG using Group Additivity
CH2OOH                  C   1H   3O   2     G   300.000  5000.000
995.043    1
 7.35066358E+00 7.88965003E-03-2.90457558E-06 4.73945953E-10-
2.85925374E-14    2
 4.65513017E+03-1.28606414E+01 3.81303407E+00 1.21039003E-02
5.82748261E-06    3
-1.54831465E-08 6.51982218E-12 5.85453866E+03 6.67808529E+00
4

!Estimated by RMG using Group Additivity
HOCHOOH                 C   1H   3O   3     G   300.000  5000.000
995.043    1
 8.41378224E+00 9.44340860E-03-4.76023706E-06 9.30384175E-10-
6.26299233E-14    2
-1.61374330E+04-1.21719999E+01 4.54350726E+00 2.03655498E-02-
1.42362974E-05    3
 2.59683778E-09 6.95111108E-13-1.51377035E+04 7.63388167E+00
4

 !Estimated by RMG using Group Additivity
C4H5-114                C   4H   5          G   300.000  5000.000
995.043    1
 7.97357483E+00 1.40708825E-02-4.35092439E-06 6.21445335E-10-
3.39054041E-14    2
 4.10439339E+04-1.40027178E+01 3.38700915E+00 1.73504782E-02
1.35555484E-05    3
-2.66851509E-08 1.06731899E-11 4.27071075E+04 1.18727483E+01
4
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!Estimated by RMG using Group Additivity
C5H9_2_4                C   5H   9          G   300.000  5000.000
995.043    1
 8.87567024E+00 2.65752556E-02-9.40610500E-06 1.50678609E-09-
8.99617643E-14    2
 1.61973506E+04-1.56961340E+01 3.73284894E+00 2.16282196E-02
3.66740871E-05    3
-5.52431102E-08 2.06696029E-11 1.84891870E+04 1.54628979E+01
4

!Estimated by RMG using Group Additivity
CHCHCH2OH               C   3H   5O   1     G   300.000  5000.000
995.043    1
 8.28958473E+00 1.35530091E-02-4.86866794E-06 7.91161885E-10-
4.77386619E-14    2
 1.11351750E+04-1.42415322E+01 3.80104915E+00 1.55129739E-02
1.64223647E-05    3
-2.97178507E-08 1.16988141E-11 1.28246599E+04 1.13917247E+01
4

!Estimated by RMG using Group Additivity
CCCC(OO)OH              C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.55312243E+01 2.49167356E-02-9.15259672E-06 1.50834317E-09-
9.18720103E-14    2
-3.66786205E+04-4.73648865E+01 3.48090553E+00 4.88222887E-02-
8.20243052E-06    3
-2.39091940E-08 1.25202678E-11-3.30658439E+04 1.68146082E+01
4

!Estimated by RMG using Group Additivity
CcCC(OOH)OH             C   4H   9O   3     G   300.000  5000.000
995.043    1
 1.47788882E+01 2.65790012E-02-1.00923700E-05 1.69541566E-09-
1.04527470E-13    2
-3.12164929E+04-4.07218569E+01 3.70276247E+00 5.08866063E-02-
1.62579128E-05    3
-1.45933111E-08 9.11826517E-12-2.80113656E+04 1.76883527E+01
4

!Primary Thermo Library: Lee&Bozzelli_JPCA_107_19_3778 (Species ID:
HOOCH2CO)
HOOCH2CO                C   2H   3O   3     G   250.000  5000.000
995.043    1
 1.21252247E+01 7.59581551E-03-2.79414296E-06 4.59496410E-10-
2.78951002E-14    2
-1.46078555E+04-3.19654955E+01 3.50376351E+00 2.29105807E-02
3.27813866E-06    3
-2.31449536E-08 1.08109717E-11-1.19345317E+04 1.43969756E+01
4

END


REACTIONS
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! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
!
! Following reactions and reaction rate expressions from GRI-Mech 3.0
mechanism,
!    unless otherwise noted

O+O+M=O2+M                                1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/
.83/
O+H+M=OH+M                               5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2=H+OH                                3.870E+04    2.700    6260.00
O+HO2=OH+O2                              2.000E+13     .000        .00
O+H2O2=OH+HO2                            9.630E+06    2.000    4000.00
O+CH=H+CO                                5.700E+13     .000        .00
O+CH2=H+HCO                              8.000E+13     .000        .00
O+CH2(S)=H2+CO                           1.500E+13     .000        .00
O+CH2(S)=H+HCO                           1.500E+13     .000        .00
!O+CH3=H+CH2O                             5.060E+13     .000        .00
O+CH4=OH+CH3                             1.020E+09    1.500    8600.00
O+CO(+M)=CO2(+M)                         1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/
.50/
!O+HCO=OH+CO                              3.000E+13     .000        .00
!O+HCO=H+CO2                              3.000E+13     .000        .00
O+CH2O=OH+HCO                            3.900E+13     .000    3540.00
O+CH2OH=OH+CH2O                          1.000E+13     .000        .00
!O+CH3O=OH+CH2O                           1.000E+13     .000        .00
O+CH3OH=OH+CH2OH                         3.880E+05    2.500    3100.00
O+CH3OH=OH+CH3O                          1.300E+05    2.500    5000.00
O+C2H=CH+CO                              5.000E+13     .000        .00
O+C2H2=H+HCCO                            1.350E+07    2.000    1900.00
O+C2H2=OH+C2H                            4.600E+19   -1.410   28950.00
O+C2H2=CO+CH2                            6.940E+06    2.000    1900.00
!O+C2H3=H+CH2CO                           3.000E+13     .000        .00
O+C2H4=CH3+HCO                           1.250E+07    1.830     220.00
!O+C2H5=CH3+CH2O                          2.240E+13     .000        .00
O+C2H6=OH+C2H5                           8.980E+07    1.920    5690.00
O+HCCO=H+CO+CO                             1.000E+14     .000        .00
O+CH2CO=OH+HCCO                          1.000E+13     .000    8000.00
!O+CH2CO=CH2+CO2                          1.750E+12     .000    1350.00
O2+CO=O+CO2                              2.500E+12     .000   47800.00
O2+CH2O=HO2+HCO                          1.000E+14     .000   40000.00
H+O2+M=HO2+M                             2.800E+18    -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/
H+O2+O2=HO2+O2                             2.080E+19   -1.240        .00
H+O2+H2O=HO2+H2O                         11.26E+18    -.760        .00
H+O2+N2=HO2+N2                           2.600E+19   -1.240        .00
H+O2+AR=HO2+AR                           7.000E+17    -.800        .00

!H+O2=O+OH                                2.650E+16    -.6707  17041.00
H+O2=O+OH   1.175E+16   -0.591      16198.00
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!From Miller, Pilling, and Troe (Proc. Combust. Inst. 2005 43-88)

H+H+M=H2+M                                1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
H+H+H2=H2+H2                                 9.000E+16    -.600        .00
H+H+H2O=H2+H2O                            6.000E+19   -1.250        .00
H+H+CO2=H2+CO2                            5.500E+20   -2.000        .00
H+OH+M=H2O+M                             2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/
H+HO2=O+H2O                              3.970E+12     .000     671.00
H+HO2=O2+H2                              4.480E+13     .000    1068.00
!H+HO2=OH+OH                                0.840E+14     .000     635.00
H+H2O2=HO2+H2                            1.210E+07    2.000    5200.00
H+H2O2=OH+H2O                            1.000E+13     .000    3600.00
H+CH=C+H2                                1.650E+14     .000        .00
H+CH2(+M)=CH3(+M)                        6.000E+14     .000        .00
     LOW  /  1.040E+26   -2.760   1600.00/
     TROE/   .5620  91.00  5836.00  8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH2(S)=CH+H2                           3.000E+13     .000        .00
H+CH3(+M)=CH4(+M)                        13.90E+15    -.534     536.00
     LOW  /  2.620E+33   -4.760   2440.00/
     TROE/   .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH4=CH3+H2                             6.600E+08    1.620   10840.00
H+HCO(+M)=CH2O(+M)                       1.090E+12     .480    -260.00
     LOW  /  2.470E+24   -2.570    425.00/
     TROE/   .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
!H+HCO=H2+CO                              7.340E+13     .000        .00
H+CH2O(+M)=CH2OH(+M)                     5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/   .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)=CH3O(+M)                      5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/   .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/

!H+CH2O=HCO+H2                            5.740E+07    1.900    2742.00
H+CH2O=HCO+H2     1.10E+08    1.77  2999.5
! Tsang, W.; Hampson, R.F., "Chemical kinetic database for combustion
chemistry.  Part I.
!    Methane and related compounds", J. Phys. Chem. Ref. Data, (1986)
v.15 1087-1279
! Discussion on p.1138, Entry (12,4): Authors note that all low
temperature results are in
!    good agreement.  Authors further state that their recommendation is
a factor of 3 higher
!    than those reported by Deen et al. (1980), measured at 1700-2500 K.
! To account for this factor of 3 discrepancy at higher T, this study
divides the recommended
!    pre-exponential factor by 2

H+CH2OH(+M)=CH3OH(+M)                    1.055E+12     .500      86.00
     LOW  /  4.360E+31   -4.650   5080.00/
     TROE/   .600  100.00  90000.0  10000.0 /
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H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH=H2+CH2O                          2.000E+13     .000        .00
!H+CH2OH=OH+CH3                           1.650E+11     .650    -284.00
H+CH2OH=CH2(S)+H2O                       3.280E+13    -.090     610.00
H+CH3O(+M)=CH3OH(+M)                     2.430E+12     .515      50.00
     LOW  /  4.660E+41   -7.440   14080.0/
     TROE/   .700  100.00  90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
!H+CH3O=H+CH2OH                           4.150E+07    1.630    1924.00
H+CH3O=H2+CH2O                           2.000E+13     .000        .00
!H+CH3O=OH+CH3                            1.500E+12     .500    -110.00
H+CH3O=CH2(S)+H2O                        2.620E+14    -.230    1070.00
!H+CH3OH=CH2OH+H2                         1.700E+07    2.100    4870.00
!H+CH3OH=CH3O+H2                          4.200E+06    2.100    4870.00
CH3OH+H=CH3O+H2 3.600E+12 0.000 6.095E+03
CH3OH+H=CH2OH+H2 1.204E+06 2.400 2.583E+03

H+C2H(+M)=C2H2(+M)                       1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/   .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/

!H+C2H2(+M)=C2H3(+M)                      5.600E+12     .000    2400.00
!     LOW  /  3.800E+40   -7.270   7220.00/
!     TROE/   .7507   98.50  1302.00  4167.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
! Rate expression from Marinov ethanol oxidation mechanism implemented;
see below.

H+C2H3(+M)=C2H4(+M)                      6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
     TROE/   .7820  207.50  2663.00  6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3=H2+C2H2                           3.000E+13     .000        .00
H+C2H4(+M)=C2H5(+M)                      0.540E+12     .454    1820.00
     LOW  /  0.600E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00  4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/

H+C2H4=C2H3+H2                           2.325E+06    2.530   12240.00
! Estimate: This study multiplies the pre-exponential factor by 2, in
better agreement with
! the rate expression reported by:
! Baulch, D.L.; Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.;
Kerr, J.A.; Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.,
!    "Evaluated kinetic data for combustion modeling", J. Phys. Chem.
Ref. Data, (1992) v.21 411-734
! Discussion on p.529

H+C2H5(+M)=C2H6(+M)                      5.210E+17    -.990    1580.00
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00  6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H5=H2+C2H4                           2.000E+12     .000        .00
H+C2H6=C2H5+H2                           1.150E+08    1.900    7530.00
H+HCCO=CH2(S)+CO                         1.000E+14     .000        .00
H+CH2CO=HCCO+H2                          5.000E+13     .000    8000.00
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!H+CH2CO=CH3+CO                          1.130E+14     .000    3428.00
! Estimate: This study multiplies the pre-exponential factor by 10, in
better agreement with
! the rate expressions located in the NIST online database
(kinetics.nist.gov)

H+HCCOH=H+CH2CO                          1.000E+13     .000        .00
H2+CO(+M)=CH2O(+M)                       4.300E+07    1.500   79600.00
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+H2=H+H2O                              2.160E+08    1.510    3430.00
OH+OH(+M)=H2O2(+M)                         7.400E+13    -.370        .00
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00  5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+OH=O+H2O                                3.570E+04    2.400   -2110.00
!OH+HO2=O2+H2O                           1.450E+13     .000    -500.00
! DUPLICATE
!OH+H2O2=HO2+H2O                         2.000E+12     .000     427.00
! DUPLICATE
!OH+H2O2=HO2+H2O                         1.700E+18     .000   29410.00
! DUPLICATE

!W. Tsang and R.F. Hampson; "Chemical kinetic database for combustion
chemistry.  Part I.
!     Methane and related compounds" J.Phys.Chem.Ref.Data 15 (1986)
OH+H2O2=HO2+H2O         1.75E+12    0.0   320.0

OH+C=H+CO                                5.000E+13     .000        .00
OH+CH=H+HCO                              3.000E+13     .000        .00
OH+CH2=H+CH2O                            2.000E+13     .000        .00
OH+CH2=CH+H2O                            1.130E+07    2.000    3000.00
OH+CH2(S)=H+CH2O                         3.000E+13     .000        .00
OH+CH3(+M)=CH3OH(+M)                     2.790E+18   -1.430    1330.00
     LOW  /  4.000E+36   -5.920   3140.00/
     TROE/   .4120  195.0  5900.00  6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3=CH2+H2O                           5.600E+07    1.600    5420.00
OH+CH3=CH2(S)+H2O                        6.440E+17   -1.340    1417.00

! MRH (26APR2010) : Changed from GRI-Mech 3.0 to Srinivasan et al.
(J.Phys.Chem.A 109 1857-1863)
OH+CH4=CH3+H2O          1.01e+06    2.18  2447.42
!OH+CH4=CH3+H2O                           1.000E+08    1.600    3120.00

OH+CO=H+CO2                              4.760E+07    1.228      70.00
OH+HCO=H2O+CO                            5.000E+13     .000        .00

OH+CH2O=HCO+H2O                          1.430E+09    1.180    -447.00
! Estimate: This study divides the pre-exponential factor by 3

OH+CH2OH=H2O+CH2O                        5.000E+12     .000        .00
OH+CH3O=H2O+CH2O                         5.000E+12     .000        .00
OH+CH3OH=CH2OH+H2O                       1.440E+06    2.000    -840.00
OH+CH3OH=CH3O+H2O                        6.300E+06    2.000    1500.00
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OH+C2H=H+HCCO                           2.000E+13     .000        .00
OH+C2H2=H+CH2CO                         2.180E-04    4.500   -1000.00
OH+C2H2=H+HCCOH                         5.040E+05    2.300   13500.00
OH+C2H2=C2H+H2O                         3.370E+07    2.000   14000.00
OH+C2H2=CH3+CO                          4.830E-04    4.000   -2000.00
OH+C2H3=H2O+C2H2                        5.000E+12     .000        .00
OH+C2H4=C2H3+H2O                        3.600E+06    2.000    2500.00

!Baulch et al. (J.Phys.Chem.Ref.Data 21 (1992) 411-429)
OH+C2H6=C2H5+H2O        7.19e+06    2.0   865.0
!OH+C2H6=C2H5+H2O                       3.540E+06    2.120     870.00

OH+CH2CO=HCCO+H2O                       7.500E+12     .000    2000.00
HO2+HO2=O2+H2O2                           1.300E+11     .000   -1630.00
 DUPLICATE
HO2+HO2=O2+H2O2                           4.200E+14     .000   12000.00
 DUPLICATE
HO2+CH2=OH+CH2O                         2.000E+13     .000        .00

HO2+CH3=O2+CH4    3.61e+12    0.0   0.0
!HO2+CH3=O2+CH4                          1.000E+12     .000        .00

!HO2+CH3=OH+CH3O                         3.780E+13     .000        .00
!HO2+CH3=OH+CH3O  1.8E+13     0.0   0.0
! Baulch, D.L.; Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.;
Kerr, J.A.; Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.,
!    "Evaluated kinetic data for combustion modeling", J. Phys. Chem.
Ref. Data, (1992) v.21 411-734
! Discussion on p.608
HO2+CH3=OH+CH3O   1.00E+12    0.2688      -688.0
! Jasper, Klippenstein, and Harding (Proc. Combust. Inst. 2009 279-286)

HO2+CO=OH+CO2                           1.500E+14     .000   23600.00

!Q.S. Li, X. Zhang, S.W. Zhang
!J.Phys.Chem.A 109 (2005) 12027-12035
HO2+CH2O=HCO+H2O2       1.89e+04    2.7   11520.0
!HO2+CH2O=HCO+H2O2                       5.600E+06    2.000   12000.00

C+O2=O+CO                               5.800E+13     .000     576.00
C+CH2=H+C2H                             5.000E+13     .000        .00
C+CH3=H+C2H2                            5.000E+13     .000        .00
CH+O2=O+HCO                             6.710E+13     .000        .00
CH+H2=H+CH2                             1.080E+14     .000    3110.00
CH+H2O=H+CH2O                           5.710E+12     .000    -755.00
CH+CH2=H+C2H2                           4.000E+13     .000        .00
CH+CH3=H+C2H3                           3.000E+13     .000        .00
CH+CH4=H+C2H4                           6.000E+13     .000        .00
CH+CO(+M)=HCCO(+M)                      5.000E+13     .000        .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+CO2=HCO+CO                           1.900E+14     .000   15792.00
CH+CH2O=H+CH2CO                         9.460E+13     .000    -515.00
CH+HCCO=CO+C2H2                         5.000E+13     .000        .00
CH2+O2=>OH+H+CO                           5.000E+12     .000    1500.00
CH2+H2=H+CH3                            5.000E+05    2.000    7230.00
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CH2+CH2=H2+C2H2                           1.600E+15     .000   11944.00
CH2+CH3=H+C2H4                          4.000E+13     .000        .00
CH2+CH4=CH3+CH3                           2.460E+06    2.000    8270.00

CH2+CO(+M)=CH2CO(+M)                    8.100E+12     .500    4510.00
     LOW  /  2.690E+33   -5.110   7095.00/
     TROE/   .5907  275.00  1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
! Estimate: This study multiplies the high pressure limit pre-
exponential factor by 10

CH2+HCCO=C2H3+CO                        3.000E+13     .000        .00
CH2(S)+N2=CH2+N2                        1.500E+13     .000     600.00
CH2(S)+AR=CH2+AR                        9.000E+12     .000     600.00
CH2(S)+O2=H+OH+CO                       2.800E+13     .000        .00
CH2(S)+O2=CO+H2O                        1.200E+13     .000        .00
CH2(S)+H2=CH3+H                         7.000E+13     .000        .00
CH2(S)+H2O(+M)=CH3OH(+M)                4.820E+17   -1.160    1145.00
     LOW  /  1.880E+38   -6.360   5040.00/
     TROE/   .6027  208.00  3922.00  10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O=CH2+H2O                      3.000E+13     .000        .00
CH2(S)+CH3=H+C2H4                       1.200E+13     .000    -570.00
CH2(S)+CH4=CH3+CH3                        1.600E+13     .000    -570.00
CH2(S)+CO=CH2+CO                        9.000E+12     .000        .00
CH2(S)+CO2=CH2+CO2                      7.000E+12     .000        .00
CH2(S)+CO2=CO+CH2O                      1.400E+13     .000        .00
CH2(S)+C2H6=CH3+C2H5                    4.000E+13     .000    -550.00
!CH3+O2=O+CH3O                           3.560E+13     .000   30480.00
CH3+O2=OH+CH2O                          2.310E+12     .000   20315.00
CH3+H2O2=HO2+CH4                        2.450E+04    2.470    5180.00

!2CH3(+M)=C2H6(+M)                        6.770E+16   -1.180     654.00
!     LOW  /  3.400E+41   -7.030   2762.00/
!     TROE/   .6190  73.20  1180.00  9999.00 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH3+CH3=C2H6      9.45E+14    -0.538      135.12
! Klippenstein, Georgievskii, Harding (Phys. Chem. Chem. Phys. 2006
1133)

CH3+CH3=H+C2H5                            6.840E+12     .100   10600.00
CH3+HCO=CH4+CO                          2.648E+13     .000        .00

CH3+CH2O=HCO+CH4                        3.320E+03    2.810    5860.00
!CH3+CH2O=HCO+CH4 7.78E-08    6.1   1969.14
! Baulch, D.L.; Cobos, C.J.; Cox, R.A.; Frank, P.; Hayman, G.; Just, T.;
Kerr, J.A.; Murrells, T.; Pilling, M.J.; Troe, J.; Walker, R.W.;
Warnatz, J.,
!    "Summary table of evaluated kinetic data for combustion modeling -
Supplement 1",
!    J. Phys. Chem. Ref. Data, (1994) v.23 847-1033
! Discussion on p.989-990

CH3+CH3OH=CH2OH+CH4                     3.000E+07    1.500    9940.00
CH3+CH3OH=CH3O+CH4                      1.000E+07    1.500    9940.00
CH3+C2H4=C2H3+CH4                       2.270E+05    2.000    9200.00
CH3+C2H6=C2H5+CH4                       6.140E+06    1.740   10450.00
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HCO+H2O=H+CO+H2O                          1.500E+18   -1.000   17000.00

! G. Friedrichs, J.T. Herbon, D.F. Davidson, R.K. Hanson
! "Quantitative detection of HCO behind shock waves: The thermal
decomposition of HCO"
! Phys. Chem. Chem. Phys. 4 (2002) 5778-5788
!HCO+M=H+CO+M     4.80E+17    -1.2  17734.23
HCO+M=H+CO+M                              1.870E+17   -1.000   17000.00
H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/

HCO+O2=HO2+CO                             13.45E+12     .000     400.00

!CH2OH+O2=HO2+CH2O                         1.800E+13     .000     900.00
CH2OH+O2=HO2+CH2O 1.21E+12    0.0   0.0
! Tsang, W.; "Chemical kinetic database for combustion chemistry.  Part
2.  Methanol"
!    J. Phys. Chem. Ref. Data, (1987) v.16 471-508
! Discussion on p.495: Entry (39,3)

CH3O+O2=HO2+CH2O                          4.280E-13    7.600   -3530.00
C2H+O2=HCO+CO                             1.000E+13     .000    -755.00
C2H+H2=H+C2H2                             5.680E+10    0.900    1993.00

! A.M. Mebel, E.W.G. Diau, M.C. Lin, K. Morokuma
! "Ab initio and RRKM calculations for multichannel rate constants of
the C2H3 + O2 reaction"
! J Am. Chem. Soc. 118 (1996) 9759-9771
!C2H3+O2=HCO+CH2O 4.58E+16    -1.39 1014.562
!Baulch et al. (J.Phys.Chem.Ref.Data 21 411 1992)
C2H3+O2=HCO+CH2O        5.42E+12    0.0   0.0
!C2H3+O2=HCO+CH2O                          4.580E+16   -1.390    1015.00

C2H4(+M)=H2+C2H2(+M)                      8.000E+12     .440   86770.00
     LOW  /  1.580E+51   -9.300  97800.00/
     TROE/   .7345  180.00  1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H5+O2=HO2+C2H4                          8.400E+11     .000    3875.00
HCCO+O2=OH+CO+CO                            3.200E+12     .000     854.00
HCCO+HCCO=CO+CO+C2H2                            1.000E+13     .000
.00
O+CH3=>H+H2+CO                              3.370E+13     .000        .00
O+C2H4=H+CH2CHO                           6.700E+06    1.830     220.00
!O+C2H5=H+CH3CHO                           1.096E+14     .000        .00

! N.K. Srinivasan, M.C. Su, J.W. Sutherland, J.V. Michael, B. Ruscic
! "Reflected shock tube studies of high-temperature rate constants for
OH+NO2=>HO2+NO and
!     OH+HO2=>H2O+O2"
! J. Phys. Chem. A 110 (2006) 6602-6607
OH+HO2=O2+H2O     3.01E+13    0.0   0.0
!OH+HO2=O2+H2O                             0.500E+16     .000   17330.00
!  DUPLICATE

OH+CH3=>H2+CH2O                             8.000E+09     .500   -1755.00
CH+H2(+M)=CH3(+M)                         1.970E+12     .430    -370.00
   LOW/ 4.820E+25  -2.80  590.0 /
   TROE/ .578  122.0  2535.0  9365.0 /
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H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+O2=>H+H+CO2                              5.800E+12     .000    1500.00
CH2+O2=O+CH2O                               2.400E+12     .000    1500.00
CH2+CH2=>H+H+C2H2                            2.000E+14     .000   10989.00
CH2(S)+H2O=>H2+CH2O                           6.820E+10     .250    -935.00

!C2H3+O2=O+CH2CHO                            3.030E+11     .290      11.00
C2H3+O2=CH2CHO+O  5.500E+14   -0.611      5.260E+03
! Marinov, N.M.; Pitz, W.J.; Westbrook, C.K.; Vincitore, A.M.; Castaldi,
M.J.; Senkan, S.M.; Melius, C.F.;,
!    "Aromatic and polycyclic aromatic hydrocarbon formation in a
laminar premixed n-butane flame",
!    Combust. Flame, (1998) v.114 192-213

C2H3+O2=HO2+C2H2                            1.337E+06    1.610    -384.00
O+CH3CHO=OH+CH2CHO                          2.920E+12     .000    1808.00
O+CH3CHO=>OH+CH3+CO                           2.920E+12     .000    1808.00
O2+CH3CHO=>HO2+CH3+CO                         3.010E+13     .000   39150.00

H+CH3CHO=CH2CHO+H2                          2.050E+08    1.160    2405.00
! Estimate: This study divides the pre-exponential factor by 10

!H+CH3CHO=>CH3+H2+CO                          2.050E+09    1.160    2405.00
!OH+CH3CHO=>CH3+H2O+CO                        2.343E+10    0.730   -1113.00
!HO2+CH3CHO=>CH3+H2O2+CO                      3.010E+12     .000   11923.00
!CH3+CH3CHO=>CH3+CH4+CO                       2.720E+06    1.770    5920.00

H+CH2CO(+M)=CH2CHO(+M)                      4.865E+11    0.422   -1755.00
    LOW/ 1.012E+42  -7.63  3854.0/
    TROE/ 0.465  201.0  1773.0  5333.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+CH2CHO=>H+CH2+CO2                           1.500E+14     .000       .00
!O2+CH2CHO=>OH+CO+CH2O                        1.810E+10     .000       .00
!O2+CH2CHO=>OH+HCO+HCO                           2.350E+10     .000
.00
!H+CH2CHO=CH3+HCO                            2.200E+13     .000       .00
H+CH2CHO=CH2CO+H2                           1.100E+13     .000       .00
OH+CH2CHO=H2O+CH2CO                         1.200E+13     .000       .00

!OH+CH2CHO=HCO+CH2OH                          3.010E+13     .000       .00
! Pressure-dependent rate expression from RMG implemented; see below

!CH3+C2H5(+M)=C3H8(+M)                        .9430E+13     .000       .00
!     LOW/ 2.710E+74  -16.82  13065.0 /
!     TROE/ .1527  291.0  2742.0  7748.0 /
!H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/



! Marinov, N.M.
!    "A detailed chemical kinetic model for high temperature ethanol
oxidation",
!    Int. J. Chem. Kinet. (1999) v.31 183-220
!
! Those reactions commented out are duplicates to the GRI-Mech 3.0
mechanism,
!     unless otherwise noted
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!OH+H2=H+H2O              2.14E+08  1.52  3449.0 !Marinov 1995a
!O+OH=O2+H                2.02E+14  -0.4     0.0 !Marinov 1995a
!O+H2=OH+H                5.06E+04  2.67  6290.0 !Marinov 1995a
!H+O2(+m)=HO2(+m)         4.52E+13  0.0      0.0 !Marinov 1995a
!   LOW / 1.05E+19  -1.257  0.0 /              !Marinov 1995a
!   H2O/0.0/ H2/0.0/ N2/0.0/ CH4/10.0/ CO2/3.8/ CO/1.9/
!H+O2(+N2)=HO2(+N2)       4.52E+13  0.0      0.0 !Marinov 1995a
!   LOW / 2.03E+20  -1.59   0.0 /                    !Marinov 1995a
!H+O2(+H2)=HO2(+H2)       4.52E+13  0.0      0.0 !Marinov 1995a
!    LOW / 1.52E+19  -1.133  0.0 /                   !Marinov 1995a
!H+O2(+H2O)=HO2(+H2O)     4.52E+13  0.0      0.0 !Marinov 1995a
!   LOW / 2.10E+23  -2.437  0.0 /              !Marinov 1995a
!OH+HO2=H2O+O2            2.13E+28 -4.827 3500.0 !Hippler 1995
!    DUPLICATE
!OH+HO2=H2O+O2           9.10E+14  0.0  10964.0 !Hippler 1995
!    DUPLICATE
!H+HO2=OH+OH              1.50E+14  0.0  1000.0  !Marinov 1995a
!H+HO2=H2+O2              6.63E+13  0.0  2126.0  !Tsang   1986x
!H+HO2=O+H2O             3.01E+13  0.0  1721.0  !Marinov 1995a
!O+HO2=O2+OH             3.25E+13  0.0     0.0  !Marinov 1995a
!OH+OH=O+H2O              3.57E+04  2.4 -2112.0  !Marinov 1995a
!H+H+m=H2+m               1.00E+18 -1.0     0.0  !Marinov 1995a
!   H2O/0.0/ H2/0.0/
!H+H+H2=H2+H2             9.20E+16 -0.6     0.0  !Marinov 1995a
!H+H+H2O=H2+H2O           6.00E+19 -1.25    0.0  !Marinov 1995a
!H+OH+m=H2O+m             2.21E+22 -2.0     0.0  !Marinov 1995a
!   H2O/6.4/
!H+O+m=OH+m               4.71E+18 -1.0     0.0  !Marinov 1995a
!   H2O/6.4/
!O+O+m=O2+m               1.89E+13  0.0 -1788.0  !Marinov 1995a
!HO2+HO2=H2O2+O2          4.20E+14  0.0 11982.0  !Marinov 1995a
!   DUPLICATE
!HO2+HO2=H2O2+O2          1.30E+11  0.0 -1629.0  !Marinov 1995a
!   DUPLICATE
!OH+OH(+m)=H2O2(+m)       1.24E+14 -0.37    0.0  !Marinov 1995a
!   LOW / 3.04E+30   -4.63   2049.0 /          !Marinov 1995a
!   TROE / 0.470   100.0   2000.0  1.0E+15 /
!H2O2+H=HO2+H2            1.98E+06  2.0  2435.0  !Marinov 1995a
!H2O2+H=OH+H2O            3.07E+13  0.0  4217.0  !Marinov 1995a
!H2O2+O=OH+HO2            9.55E+06  2.0  3970.0  !Marinov 1995a
!H2O2+OH=H2O+HO2          2.40E+00 4.042 -2162.0 !Marinov 1995a
!CH3+CH3(+m)=C2H6(+m)     9.22E+16 -1.174 636.0  !Walter  1990
!   LOW / 1.14E+36   -5.246  1705.0 /          !Walter  1990
!   TROE / 0.405  1120.0     69.6  1.0E+15 /
!   H2O/5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH3+H(+m)=CH4(+m)        2.14E+15 -0.4    0.0   !Tsang 1986
!   LOW /  3.31E+30   -4.0  2108.0 /                !Marinov 1996
!   TROE / 0.0   1.0E-15   1.0E-15   40.0 /
!   H2O/5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH4+H=CH3+H2             2.20E+04 3.0   8750.0  !Miller 1992
!CH4+OH=CH3+H2O             4.19E+06 2.0   2547.0  !Marinov 1995
!CH4+O=CH3+OH               6.92E+08 1.56  8485.0  !Marinov 1995
!CH4+HO2=CH3+H2O2         1.12E+13 0.0   24640.0 !Marinov 1995
!CH3+HO2=CH3O+OH          7.00E+12 0.0      0.0  !Troe  1993
!CH3+HO2=CH4+O2       3.00E+12 0.0      0.0  !Marinov 1995
!CH3+O=CH2O+H         8.00E+13 0.0      0.0  !Marinov 1995
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!CH3+O2=CH3O+O       1.45E+13 0.0   29209.0 !Klatt 1991
!CH3+O2=CH2O+OH            2.51E+11 0.0   14640.0 !Marinov 1995
!CH3O+H=CH3+OH           1.00E+13 0.0      0.0  !Marinov 1998
!CH2OH+H=CH3+OH          1.00E+13 0.0      0.0  !Marinov 1998
!CH3+OH=CH2(S)+H2O       2.00E+13 0.0    550.0  !Pilling 1997
!CH3+OH=HCOH+H2          1.00E+10 0.0   -415.0  !Pilling 1997
!CH3+OH=CH2+H2O          3.00E+06 2.0   2500.0  !Marinov 1996
!CH3+H=CH2+H2            9.00E+13 0.0   15100.0 !Miller 1992
!CH3+m=CH+H2+m           6.90E+14 0.0   82469.0 !Markus 1992
!CH3+m=CH2+H+m           1.90E+16 0.0   91411.0 !Markus 1992
!CH3+OH(+m)=CH3OH(+m)    8.70E+13 0.1       0.0 !Fagerstrom 1993
!   LOW/ 8.84E+41   -7.4   626.0 /          !Marinov 1996
!   TROE /  0.025   1.0E-15   8000.0   3000.0/
!   H2O /10.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH3OH(+m)=CH2(S)+H2O(+m)  2.837e10 1.0 83871.     !Marinov 1998
!   LOW / 1.78e49 -8.81 93369./
!   TROE /0.9 740. 980. 5100./
!   H2O/10.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH3OH(+m)=HCOH+H2(+m) 4.2e9 1.12 85604.           !Marinov 1998
!    LOW / 5.02e47 -8.402 94823./
!    TROE/ 0.9 615. 915. 4615./
!    H2O /10.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH3OH(+m)=CH2O+H2(+m) 2.03e9 1.0 91443.           !Marinov 1998
!   LOW /9.784e47 -8.4 101761./
!   TROE/ 0.9 825. 1125. 5700./
!   H2O/10.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!CH3OH+OH=CH2OH+H2O      2.61E+05  2.182 -1344.0   !Tsang  1987
!CH3OH+OH=CH3O+H2O       2.62E+06  2.056   916.0   !Tsang  1987
!CH3OH+O=CH2OH+OH        3.88E+05  2.5    3080.0   !Tsang  1987
!CH3OH+H=CH2OH+H2        1.70E+07  2.1    4868.0   !Tsang  1987
!CH3OH+H=CH3O+H2         4.24E+06  2.1    4868.0   !Tsang  1987
!CH3OH+CH3=CH2OH+CH4     3.19E+01  3.17   7171.0   !Tsang  1987
!CH3OH+CH3=CH3O+CH4      1.45E+01  3.10   6935.0   !Tsang  1987
!CH3OH+HO2=CH2OH+H2O2     9.64E+10  0.0   12578.0   !Tsang  1987
CH2OH+H2O2=HO2+CH3OH    3.01E+09    0.0   2580.0      !Tsang 1987
!CH2O+H(+m)=CH3O(+m)     5.40E+11  0.454  2600.0   !GRI-Mech2.11
!   LOW/ 1.50E+30 -4.80 5560./
!   TROE/ 0.758 94. 1555. 4200./
!   H2O/5.0/
!CH2O+H(+m)=CH2OH(+m)    5.40E+11  0.454  3600.0   !GRI-Mech2.11
!   LOW / 9.10E+31 -4.82 6530./
!   TROE/ 0.7187 103. 1291. 4160./
!   H2O/5.0/
!CH3O+CH3=CH2O+CH4       1.20E+13  0.0      0.0   !Tsang  1986
!CH3O+H=CH2O+H2          2.00E+13  0.0      0.0   !Miller 1992
!CH2OH+H=CH2O+H2         2.00E+13  0.0      0.0   !Miller 1992
!CH3O+OH=CH2O+H2O        1.00E+13  0.0      0.0   !Miller 1992
!CH2OH+OH=CH2O+H2O       1.00E+13  0.0      0.0   !Miller 1992
!CH3O+O=CH2O+OH          1.00E+13  0.0      0.0   !Miller 1992
!CH2OH+O=CH2O+OH         1.00E+13  0.0      0.0   !Miller 1992
!CH3O+O2=CH2O+HO2        6.30E+10  0.0   2600.0   !Miller 1992
!CH3O+CO=CH3+CO2         4.68E+02  3.16  5380.0   !Wantuck 1987
!CH2OH+O2=CH2O+HO2       1.57E+15  -1.0     0.0   !Baulch 1992
!   DUPLICATE
!CH2OH+O2=CH2O+HO2       7.23E+13  0.0   3577.0   !Baulch 1992
!   DUPLICATE
!HCOH+OH=HCO+H2O         2.00E+13  0.0      0.0   !Marinov 1996
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!HCOH+H=CH2O+H           2.00E+14  0.0      0.0   !Marinov 1996
!HCOH+O=CO+OH+H          8.00E+13  0.0      0.0   !Marinov 1996
!HCOH+O2=CO+OH+OH        1.00E+13  0.0      0.0   !Marinov 1998
!HCOH+O2=CO2+H2O         1.00E+13  0.0      0.0   !Marinov 1998
!HCOH=CH2O               2.10E+19 -3.07 31700.0   !Marinov 1998
!CH2+H=CH+H2             1.00E+18  -1.56    0.0   !Miller 1992
!CH2+OH=CH+H2O           1.13E+07  2.0   3000.0   !Miller 1992
!CH2+OH=CH2O+H           2.50E+13  0.0      0.0   !Miller 1992
CH2+CO2=CH2O+CO         1.10E+11  0.0   1000.0   !Miller 1992
!CH2+O=CO+H+H            5.00E+13  0.0      0.0   !Miller 1992
!CH2+O=CO+H2             3.00E+13  0.0      0.0   !Miller 1992
!CH2+O2=CH2O+O           3.29E+21 -3.3   2868.0   !Marinov 1996
!CH2+O2=CO2+H+H          3.29E+21 -3.3   2868.0   !Marinov 1996
CH2+O2=CO2+H2           1.01E+21 -3.3   1508.0   !Marinov 1996
CH2+O2=CO+H2O           7.28E+19 -2.54  1809.0   !Marinov 1996
CH2+O2=HCO+OH           1.29E+20 -3.3    284.0   !Marinov 1996
!CH2+CH3=C2H4+H          4.00E+13  0.0      0.0   ! Miller 1992
!CH2+CH2=C2H2+H+H        4.00E+13  0.0      0.0   ! Miller 1992
!CH2+HCCO=C2H3+CO        3.00E+13  0.0      0.0   ! Miller 1992
CH2+C2H2=pC3H3+H       1.20E+13  0.0   6600.0   ! Miller 1992
CH2(S)+m=CH2+m          1.00E+13  0.0      0.0   ! Miller 1992
   H /12.0/ C2H2 /4.0/ H2O/3.0/
!CH2(S)+CH4=CH3+CH3      4.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+C2H6=CH3+C2H5    1.20E+14  0.0      0.0   ! Miller 1992
!CH2(S)+O2=CO+OH+H       7.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+H2=CH3+H         7.00E+13  0.0      0.0   ! Miller 1992
CH2(S)+C2H2=pC3H3+H     1.50E+14  0.0      0.0   ! Canosa-Mas85
CH2(S)+C2H4=aC3H5+H     1.30E+14  0.0      0.0   ! Canosa-Mas85
!CH2(S)+O=CO+H+H         3.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+OH=CH2O+H        3.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+H=CH+H2          3.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+CO2=CH2O+CO      3.00E+12  0.0      0.0   ! Miller 1992
!CH2(S)+CH3=C2H4+H       2.00E+13  0.0      0.0   ! Miller 1992
!CH2(S)+CH2CO=C2H4+CO    1.60E+14  0.0      0.0   ! Miller 1992
!CH+O2=HCO+O             3.30E+13  0.0      0.0   ! Miller 1992
!CH+O=CO+H               5.70E+13  0.0      0.0   ! Miller 1992
!CH+OH=HCO+H             3.00E+13  0.0      0.0   ! Miller 1992
!CH+CO2=HCO+CO           3.40E+12  0.0    690.0   ! Miller 1992
!CH+H2O=CH2O+H           1.17E+15  -0.75    0.0   ! Miller 1992
!CH+CH2O=CH2CO+H         9.46E+13  0.0   -515.0   ! Miller 1992
CH+C2H2=C3H2+H          1.00E+14  0.0      0.0   ! Miller 1992
!CH+CH2=C2H2+H           4.00E+13  0.0      0.0   ! Miller 1992
!CH+CH3=C2H3+H           3.00E+13  0.0      0.0   ! Miller 1992
!CH+CH4=C2H4+H           6.00E+13  0.0      0.0   ! Miller 1992
HCOOH+m=CO+H2O+m        2.09E+14   0.0   40400.0 !Saito 1984
HCOOH+m=CO2+H2+m        1.35E+15   0.0   60600.0 !Saito 1984
HCOOH+OH=>CO2+H2O+H       2.62E+6    2.056   916.0 !Marinov 1998
HCOOH+OH=>CO+H2O+OH       1.85E+7    1.5    -962.0 !Marinov 1998
HCOOH+H=>CO2+H2+H         4.24E+6    2.1    4868.0 !Marinov 1998
HCOOH+H=>CO+H2+OH         6.06E+13  -0.35   2988.0 !Marinov 1998
HCOOH+CH3=>CH4+CO+OH      3.90E-7    5.8    2200.0 !Marinov 1998
HCOOH+HO2=>CO+H2O2+OH     2.40E+19  -2.2   14030.0 !Marinov 1998
HCOOH+O=>CO+OH+OH         1.77E+18  -1.9    2975.0 !Marinov 1998
!CH2O+OH=HCO+H2O         3.43E+09  1.18  -447.0   ! Tsang  1986
!CH2O+H=HCO+H2           2.19E+08  1.77  3000.0   ! Miller 1992
!CH2O+m=HCO+H+m          3.31E+16  0.0   81000.0  ! Miller 1992
!CH2O+O=HCO+OH           1.80E+13  0.0   3080.0   ! Miller 1992
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!HCO+O2=CO+HO2           7.58E+12  0.0    410.0   ! Timonen 1988
!HCO+m=H+CO+m            1.86E+17  -1.0 17000.0   ! Timonen 1987
!   H2O/5.0/ H2/1.87/ CO2/3.0/ CO/1.87/ CH4/2.81/
!HCO+OH=H2O+CO           1.00E+14  0.0     0.0    ! Miller 1992
!HCO+H=CO+H2             1.19E+13  0.25    0.0    ! Miller 1992
!HCO+O=CO+OH         3.00E+13  0.0     0.0    ! Miller 1992
!HCO+O=CO2+H             3.00E+13  0.0     0.0    ! Miller 1992
!CO+OH=CO2+H             9.42E+03  2.25 -2351.0   !Marinov 1996
!CO+O+m=CO2+m            6.17E+14  0.0   3000.0   ! Miller 1992
!CO+O2=CO2+O             2.53E+12  0.0  47688.0   ! Miller 1992
!CO+HO2=CO2+OH           5.80E+13  0.0  22934.0   ! Miller 1992
!C2H5OH(+m)=CH3+CH2OH(+m) 5.94E+23 -1.68 91163.0  !Marinov 1998
!   LOW /2.88E+85 -18.9 109914./
!   TROE/0.5 200. 890.  4600./
!   H2O/5./ H2/2.0/ CO2/3.0/ CO/2.0/
!C2H5OH(+m)=C2H5+OH(+m)  1.25E+23 -1.54 96005.0   !Marinov 1998
!   LOW /3.252E+85 -18.81 114930./
!   TROE/0.5 300. 900. 5000./
!   H2O/5./ H2/2.0/ CO2/3.0/ CO/2.0/
!C2H5OH(+m)=C2H4+H2O(+m)  2.79E+13 0.09  66136.0   !Marinov 1998
!    LOW/2.57E+83 -18.85 86452./
!    TROE/0.70 350. 800. 3800./
!    H2O/5./
!C2H5OH(+m)=CH3CHO+H2(+m) 7.24E+11 0.095  91007.0   !Marinov 1998
!    LOW /4.46e87 -19.42 115586./
!    TROE/0.9 900. 1100. 3500./
!    H2O/5./
!C2H5OH+OH=C2H5O-1+H2O     1.74E+11   0.27    600.0 !Marinov 1998
C2H5OH+OH=C2H5O-2+H2O    4.64E+11   0.15      0.0 !Marinov 1998
!C2H5OH+OH=C2H5O-3+H2O    7.46E+11   0.30   1634.0 !Marinov 1998
C2H5OH+H=C2H5O-1+H2       1.23E+7    1.8    5098.0 !Marinov 1998
C2H5OH+H=C2H5O-2+H2      2.58E+7    1.65   2827.0 !Marinov 1998
C2H5OH+H=C2H5O-3+H2      1.50E+7    1.60   3038.0 !Marinov 1998
!C2H5OH+O=C2H5O-1+OH       9.41E+7    1.70   5459.0 !Marinov 1998
!C2H5OH+O=C2H5O-2+OH      1.88E+7    1.85   1824.0 !Marinov 1998
!C2H5OH+O=C2H5O-3+OH      1.58E+7    2.00   4448.0 !Marinov 1998
C2H5OH+CH3=C2H5O-1+CH4    2.19E+2    3.18   9622.0 !Marinov 1998
C2H5OH+CH3=C2H5O-2+CH4   7.28E+2    2.99   7948.0 !Marinov 1998
C2H5OH+CH3=C2H5O-3+CH4   1.45E+2    2.99   7649.0 !Marinov 1998
C2H5OH+HO2=C2H5O-2+H2O2  8.20E+3    2.55  10750.0 !Marinov 1998
!C2H5OH+HO2=C2H5O-1+H2O2   1.23E+4    2.55  15750.0 !Marinov 1998
!C2H5OH+HO2=C2H5O-3+H2O2  2.50E+12   0.0   24000.0 !Marinov 1998
!C2H5O-3+m=CH3CHO+H+m     1.16E+35  -5.89  25274.0 !Marinov 1998
!C2H5O-3+m=CH3+CH2O+m     1.35E+38  -6.96  23800.0 !Marinov 1998
C2H5O-3+O2=CH3CHO+HO2    4.00E+10   0.0    1100.0 !Hartmann 1990
!C2H5O-3+CO=C2H5+CO2      4.68E+2    3.16   5380.0 !Marinov 1998
!C2H5O-3+H=CH3+CH2OH      3.00E+13   0.0       0.0 !Marinov 1998
!C2H5O-3+H=C2H4+H2O       3.00E+13   0.0       0.0 !Marinov 1998
!C2H5O-3+OH=CH3CHO+H2O    1.00E+13   0.0       0.0 !Marinov 1998
!C2H5O-2+O2=CH3CHO+HO2    4.82E+14   0.0    5017.0 !Marinov 1998
!   DUPLICATE
!C2H5O-2+O2=CH3CHO+HO2    8.43E+15  -1.2       0.0 !Marinov 1998
!   DUPLICATE
C2H5O-2+CH3=C3H6+H2O     1.00E+13   0.0       0.0 !Marinov 1998
C2H5O-2+O=CH3CHO+OH      1.00E+14   0.0       0.0 !Marinov 1998
!C2H5O-2+H=C2H4+H2O       3.00E+13   0.0       0.0 !Marinov 1998
!C2H5O-2+H=CH3+CH2OH      3.00E+13   0.0       0.0 !Marinov 1998
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C2H5O-2+HO2=CH3CHO+OH+OH 4.00E+13   0.0       0.0 !Marinov 1998
C2H5O-2+OH=CH3CHO+H2O    5.00E+12   0.0       0.0 !Marinov 1998
!C2H5O-2+m=CH3CHO+H+m     1.00E+14   0.0   25000.0 !Marinov 1998
CH3CHO+OH=CH3CO+H2O      9.24E+6    1.5    -962.0 !Taylor 1996

CH3CHO+OH=CH2CHO+H2O     1.72E+5    2.4     2815.0 !Taylor 1996
! Estimate: This study increased the activation energy by 2 kcal/mol

CH3CHO+OH=CH3+HCOOH      3.00E+15  -1.076     0.0 !Marinov 1998
CH3CHO+O=CH3CO+OH        1.77E+18  -1.9    2975.0 !Marinov 1998
!CH3CHO+O=CH2CHO+OH       3.72E+13  -0.2    3556.0 !Marinov 1998

!CH3CHO+H=CH3CO+H2        4.66E+13  -0.35   2988.0 !Marinov 1998
CH3CHO+H=CH3CO+H2 4.100E+09   1.16  2405.0
! Estimate: This study assumes the total H+CH3CHO=products rate
expression from:
! Baulch, D.L.; Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.;
Kerr, J.A.; Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.,
!    "Evaluated kinetic data for combustion modeling", J. Phys. Chem.
Ref. Data, (1992) v.21 411-734
! Discussion on p.539

!CH3CHO+H=CH2CHO+H2       1.85E+12   0.40   5359.0 !Marinov 1998

CH3CHO+CH3=CH3CO+CH4     0.90E-7    5.8    2200.0 !Marinov 1998
!Estimate: This study divides the pre-exponential factor by 4

CH3CHO+CH3=CH2CHO+CH4    2.45E+1    3.15   5727.0 !Marinov 1998
CH3CHO+HO2=CH3CO+H2O2    2.40E+19  -2.2   14030.0 !Marinov 1998
CH3CHO+HO2=CH2CHO+H2O2   2.32E+11   0.40  14864.0 !Marinov 1998
CH3CHO+O2=CH3CO+HO2      1.00E+14   0.00  42200.0 ! xxxxx
!C2H6+CH3=C2H5+CH4       5.50E-01  4.0   8300.0   ! Miller 1992
!C2H6+H=C2H5+H2          5.40E+02  3.5   5210.0   ! Miller 1992
!C2H6+O=C2H5+OH          3.00E+07  2.0   5115.0   ! Miller 1992
!C2H6+OH=C2H5+H2O        7.23E+06  2.0    864.0   ! Baulch 1992
!C2H5+H=C2H4+H2          1.25E+14  0.0   8000.0   ! Marinov 1995
!C2H5+H=CH3+CH3          3.00E+13  0.0      0.0   ! Warnatz 1984
!C2H5+H=C2H6             3.00E+13  0.0      0.0   ! Marinov 1998
!C2H5+OH=C2H4+H2O        4.00E+13  0.0      0.0   ! Marinov 1995
!C2H5+O=CH3+CH2O         1.00E+14  0.0      0.0   ! Herron 1988
C2H5+HO2=C2H6+O2        3.00E+12  0.0      0.0   ! Marinov 1998
C2H5+HO2=C2H5O-3+OH     3.00E+13  0.0      0.0   ! Tsang 1986
!C2H5+O2=C2H4+HO2         2.89E+28  -5.4  7585.0   ! Marinov 1998
C2H5+O2=CH3CHO+OH       4.90E+11 -0.48  8357.0   ! Marinov 1998
!C2H4+OH=C2H5O-1          1.29E+12  0.0    -817.0  ! Atkinson 1986
C2H5O-1+O2=HOC2H4O2      1.00E+12  0.0   -1100.0  ! Marinov 1998
HOC2H4O2=CH2O+CH2O+OH   6.00E+10  0.0   24500.0  ! Marinov 1998
!C2H4+OH=C2H3+H2O         2.02E+13  0.0   5936.0   ! Miller 1992
!C2H4+O=CH3+HCO             1.02E+07  1.88   179.0   ! Baulch 1994
!C2H4+O=CH2CHO+H          3.39E+06  1.88   179.0   ! Baulch 1994
!C2H4+CH3=C2H3+CH4        6.62E+00  3.7   9500.0   ! Marinov 1995
!C2H4+H=C2H3+H2           3.36E-07  6.0   1692.0   ! Dagaut 1990
!C2H4+H(+m)=C2H5(+m)    1.08E+12  0.454 1822.0   ! Feng  1993
!   LOW / 1.112E+34  -5.0    4448.0 /                 ! Marinov 1996
!   TROE / 1.0   1.0E-15   95.0  200.0 /
!   H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!C2H4(+m)=C2H2+H2(+m)    1.8e14  0.0  87000.      ! Marinov 1997
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!   LOW / 1.5e15 0.0  55443. /
!C2H3+H(+m)=C2H4(+m)   6.1e12 0.27 280.           !GRI-Mech2.11
!   LOW/9.8e29 -3.86 3320./
!   TROE/ 0.782 208. 2663. 6095./
!   H2O/5.0/
!C2H3+H=C2H2+H2          9.00E+13  0.0      0.0   ! Tsang 1986
!C2H3+O=CH2CO+H          3.00E+13  0.0      0.0   ! Miller 1992
!C2H3+O2=CH2O+HCO        1.70E+29  -5.312 6500.0  ! Marinov 1997
!C2H3+O2=CH2CHO+O        5.50E+14  -0.611 5260.0  ! Marinov 1997
!C2H3+O2=C2H2+HO2        2.12E-06  6.0   9484.0   !cfm/nmm 1996
!C2H3+OH=C2H2+H2O        2.00E+13  0.0      0.0   ! Miller 1992
!C2H3+C2H=C2H2+C2H2      3.00E+13  0.0      0.0   ! Miller 1992
!C2H3+CH=CH2+C2H2        5.00E+13  0.0      0.0   ! Miller 1992
!C2H3+CH3=aC3H5+H        4.73E+02  3.7   5677.0   ! Marinov 1996

!C2H3+CH3=C3H6           4.46E+56 -13.0 13865.0   ! Marinov 1996
! Pressure-dependent reaction rate expression generated by RMG
implemented; see below

C2H3+CH3=C2H2+CH4       2.00E+13  0.0      0.0   ! Fahr  1991
!C2H2+OH=C2H+H2O         3.37E+07  2.0  14000.0   ! Miller 1992
!C2H2+OH=HCCOH+H         5.04E+05  2.3  13500.0   ! Miller 1992
!C2H2+OH=CH2CO+H         2.18E-04  4.5  -1000.0   ! Miller 1992
!   DUPLICATE
!C2H2+OH=CH2CO+H         2.00E+11  0.0      0.0   ! Vandooren 1977
!   DUPLICATE
!C2H2+OH=CH3+CO          4.83E-04  4.0  -2000.0   ! Miller 1992
!HCCOH+H=CH2CO+H         1.00E+13  0.0      0.0   ! Miller 1992
!C2H2+O=CH2+CO           6.12E+06  2.0   1900.0   ! Marinov 1996
!C2H2+O=HCCO+H           1.43E+07  2.0   1900.0   ! Marinov 1996
!C2H2+O=C2H+OH           3.16E+15 -0.6   15000.0  ! Miller 1992
!C2H2+CH3=C2H+CH4        1.81E+11  0.0   17289.0  ! Tsang  1986
C2H2+CH3=C2H+CH4        1.760e+04   2.607 27104 !MRH G3 calculations
C2H2+O2=HCCO+OH         4.00e+07  1.5   30100.0  ! Marinov 1997
!C2H2+m=C2H+H+m          4.20E+16  0.0  107000.0  ! Miller 1992

C2H2+H(+m)=C2H3(+m)    3.11E+12  0.58   2589.0  ! Knyazev 1995
   LOW / 2.25E+40  -7.269   6577.0 /                  ! Marinov 1996
   TROE /1.0 1.0E-15  675.0 1.0E+15 /
   H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
! Estimate: This study multiplies high pressure limit pre-exponential
factor by 10

!CH2CHO+H=CH3+HCO         5.00E+13   0.0       0.0 !Marinov 1998
!CH2CHO+H=CH2CO+H2        2.00E+13   0.0       0.0 !Marinov 1998
!CH2CHO+O=CH2O+HCO        1.00E+14   0.0       0.0 !Marinov 1996
!CH2CHO+OH=CH2CO+H2O      3.00E+13   0.0       0.0 !Marinov 1996
!CH2CHO+O2=CH2O+CO+OH     3.00E+10   0.0       0.0 !Baulch  1992
!CH2CHO+CH3=C2H5+CO+H     4.90E+14  -0.50      0.0 !Marinov 1998
!CH2CHO+HO2=CH2O+HCO+OH   7.00E+12   0.0       0.0 !Marinov 1998
CH2CHO+HO2=CH3CHO+O2     3.00E+12   0.0       0.0 !Marinov 1998
!CH2CHO=CH3+CO            1.17E+43  -9.83  43756.0 !Marinov 1998
!CH2CHO=CH2CO+H           1.81E+43  -9.61  45868.0 !Marinov 1998
!HCOCHO(+m)=CH2O+CO(+m)  4.27E+12  0.0   50600.0  ! Marinov 1995
!   LOW /  8.91E+16    0.0    49200.0 /              ! Marinov 1995
!HCOCHO=CO+CO+H2         4.07E+42 -8.5   69278.0  ! Marinov 1996
!HCOCHO+OH=HCO+CO+H2O    1.00E+13  0.0       0.0  ! Marinov 1995
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!HCOCHO+O=HCO+CO+OH      7.24E+12  0.0    1970.0  ! Marinov 1995
!HCOCHO+H=CH2O+HCO       1.00E+12  0.0       0.0  ! Marinov 1995
!HCOCHO+HO2=HCO+CO+H2O2  1.70E+12  0.0   10700.0  ! Marinov 1995
!HCOCHO+CH3=HCO+CO+CH4   1.74E+12  0.0    8440.0  ! Marinov 1995
!HCOCHO+O2=HCO+CO+HO2    1.00E+14  0.0   37000.0  ! Marinov 1995
CH3CO(+m)=CH3+CO(+m)    3.00E+12  0.0   16722.0  ! Warnatz 1984
    LOW / 1.20E+15    0.0     12518.0 /              ! Warnatz 1984
!CH2CO+O=CO2+CH2          1.75E+12  0.0    1350.0  ! Marinov 1995
!CH2CO+H=CH3+CO           2.71E+4   2.75    714.0  ! Marinov 1996
!CH2CO+H=HCCO+H2          2.00E+14  0.0    8000.0  ! Marinov 1996
!CH2CO+O=HCCO+OH          1.00E+13  0.0    8000.0  ! Miller 1992
!CH2CO+OH=HCCO+H2O        1.00E+13  0.0    2000.0  ! Marinov 1996
CH2CO+OH=CH2OH+CO        3.73E+12  0.0   -1013.0  ! Brown 1989
!CH2CO(+m)=CH2+CO(+m)    3.00E+14  0.0   70980.0  ! Miller 1992
!   LOW /  3.60E+15    0.0    59270.0 /              ! Miller 1992
!C2H+H2=C2H2+H       4.09E+05  2.39    864.3  ! Miller 1992
!C2H+O=CH+CO              5.00E+13  0.0       0.0  ! Miller 1992
!C2H+OH=HCCO+H            2.00E+13  0.        0.0  ! Miller 1992
C2H+O2=CO+CO+H           9.04E+12  0.0    -457.0  ! Opansky 1993
!HCCO+C2H2=pC3H3+CO      1.00E+11  0.0    3000.0  ! Miller 1992
!HCCO+H=CH2(S)+CO         1.00E+14  0.0       0.0  ! Miller 1992
!HCCO+O=H+CO+CO           8.00E+13  0.0       0.0  ! Peeters 1995
HCCO+O=CH+CO2            2.95E+13  0.0    1113.0  ! Peeters 1995
HCCO+O2=HCO+CO+O         2.50E+8   1.0       0.0  ! Marinov 1997
HCCO+O2=CO2+HCO          2.40E+11  0.0    -854.0  ! Marinov 1997
!HCCO+CH=C2H2+CO          5.00E+13  0.0       0.0  ! Miller 1992
!HCCO+HCCO=C2H2+CO+CO     1.00E+13  0.0       0.0  ! Miller 1992
HCCO+OH=C2O+H2O          3.00E+13  0.0       0.0  ! Miller 1992
C2O+H=CH+CO              1.00E+13  0.0       0.0  ! Miller 1992
C2O+O=CO+CO              5.00E+13  0.0       0.0  ! Miller 1992
C2O+OH=CO+CO+H           2.00E+13  0.0       0.0  ! Miller 1992
C2O+O2=CO+CO+O           2.00E+13  0.0       0.0  ! Miller 1992
!C3H8(+m)=C2H5+CH3(+m)   7.90E+22 -1.8   88629.0  ! Tsang 1988
!   LOW / 7.237E+27 -2.88 67448.0 /                 ! Al-Alami 1983
!   TROE /1.0 1.0E-15 1500.0 1.0E+15/
!   H2O/5.0/ CO2/3.0/ CO/2.0/ H2/2.0/
C3H7-2+HO2=C3H8+O2       3.00E+12  0.0       0.0  !Marinov 1998
C3H7-1+HO2=C3H8+O2       3.00E+12  0.0       0.0  !Marinov 1998
!C3H8+HO2=C3H7-1+H2O2     4.76E+04  2.55  16492.0  ! Tsang 1988
!C3H8+HO2=C3H7-2+H2O2     9.64E+03  2.6   13909.0  ! Tsang 1988
C3H8+OH=C3H7-1+H2O       3.16E+07  1.8     934.0  ! Cohen 1991
C3H8+OH=C3H7-2+H2O       7.08E+06  1.9    -159.0  ! Cohen 1991
!C3H8+O=C3H7-1+OH         3.73E+06  2.4    5504.0  ! Cohen 1986
!C3H8+O=C3H7-2+OH         5.48E+05  2.5    3139.0  ! Cohen 1986
C3H8+H=C3H7-2+H2         1.30E+06  2.4    4471.0  ! Tsang 1988
C3H8+H=C3H7-1+H2         1.33E+06  2.54   6756.0  ! Tsang 1988
C3H8+CH3=C3H7-1+CH4      9.04E-01  3.65   7153.0  ! Tsang 1988
C3H8+CH3=C3H7-2+CH4      1.51E+00  3.46   5480.0  ! Tsang 1988
!C3H8+C2H3=C3H7-2+C2H4    1.00E+03  3.1    8830.0  ! Tsang 1988
!C3H8+C2H3=C3H7-1+C2H4    6.00E+02  3.3   10500.0  ! Tsang 1988
!C3H8+C2H5=C3H7-2+C2H6    1.51E+00  3.46   7470.0  ! Tsang 1988
!C3H8+C2H5=C3H7-1+C2H6    9.03E-01  3.65   9140.0  ! Tsang 1988
!C3H8+aC3H5=C3H6+C3H7-1   2.35E+02  3.3   19842.0  ! Tsang 1988
!C3H8+aC3H5=C3H6+C3H7-2   7.83E+01  3.3   18169.0  ! Tsang 1988
!C3H7-1(+m)=C2H4+CH3(+m)  1.23E+13  -0.1  30202.0  ! Bencsura 1992
!   LOW / 5.485E+49  -10.0  35766.0 /               ! Bencsura 1992
!   TROE / 2.17   1.0E-15   251.0   1185.0 /
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!   H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
!C3H6+H(+m)=C3H7-2(+m)   5.70E+09   1.16    874.0  ! Seakins 1993
!   LOW / 1.64E+54   -11.1   9364.0 /                ! Marinov 1996
!   TROE / 1.0   1.0E-15   260.0   3000.0 /
!   H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/
C3H7-2+O2=C3H6+HO2       1.88E+20 -2.69    7109.0 ! Marinov 1998

!C3H7-1+O2=C3H6+HO2       3.83E+26  -4.44   7724.0 ! Marinov 1998
! Pressure-dependent reaction rate expression generated by RMG
implemented; see below

!C3H7-2+H=C2H5+CH3        5.00E+13   0.0       0.0 ! Tsang 1988
!C3H7-1+H=C2H5+CH3        1.00E+14   0.0       0.0 ! Tsang 1988
C3H6=C2H2+CH4           2.50E+12   0.0   70000.0 ! Hidaka 1992
C3H6=aC3H4+H2           3.00E+13   0.0   80000.0 ! Hidaka 1992
!pC3H5+H=C3H6            1.00E+14   0.0       0.0 !Marinov 1998
!sC3H5+H=C3H6            1.00E+14   0.0       0.0 !Marinov 1998
!C3H6+HO2=aC3H5+H2O2     9.64E+03   2.6   13910.0 ! Tsang 1991
aC3H5+H2O2=C3H6+HO2     2.0305      3.29  1.0725e+03  !H_Abstraction
estimate: (Average:)    C_rad/H2/Cd     H2O2          deltaHrxn(T=298K)
= -3.0695403041872 kcal/mol

!J. Zador, A.W. Jasper, J.A. Miller
!Phys.Chem.Chem.Phys. 11 (2009) 11048
!C3H6+OH=H2O+aC3H5            -1.25e+08   1.73  925
!   DUP
!C3H6+OH=H2O+aC3H5            1.88e+07    2.03  684
!   DUP
C3H6+OH=aC3H5+H2O      3.12E+06   2.0    -298.0  ! Tsang 1991

C3H6+OH=sC3H5+H2O      1.11E+06   2.0    1451.0  ! Tsang 1991
C3H6+OH=pC3H5+H2O      2.11E+06   2.0    2778.0  ! Tsang 1991
!C3H6+O=C3H4O-enone+H+H     5.01E+07   1.76     76.0  ! Tsang 1991
!C3H6+O=C2H5+HCO        1.58E+07   1.76  -1216.0  ! Tsang 1991
!C3H6+O=aC3H5+OH        5.24E+11   0.7    5884.0  ! Tsang 1991
!C3H6+O=pC3H5+OH        1.20E+11   0.7    8959.0  ! Tsang 1991
!C3H6+O=sC3H5+OH        6.03E+10   0.7    7632.0  ! Tsang 1991
!C3H6+H=C2H4+CH3        4.23E+12   0.0    1302.0  ! Tsang 1991
C3H6+H=aC3H5+H2        1.73E+05   2.5    4492.0  ! Tsang 1991
C3H6+H=sC3H5+H2        4.09E+05   2.5    9794.0  ! Tsang 1991
C3H6+H=pC3H5+H2        8.04E+05   2.5   12284.0  ! Tsang 1991
aC3H5+HO2=C3H6+O2      3.00E+12   0.0       0.0  ! Tsang 1991
C3H6+CH3=aC3H5+CH4     2.22E+00   3.5    5675.0  ! Tsang 1991
C3H6+CH3=sC3H5+CH4     8.43E-01   3.5   11656.0  ! Tsang 1991
C3H6+CH3=pC3H5+CH4     1.35E+00   3.5   12848.0  ! Tsang 1991
!C3H6+C2H5=aC3H5+C2H6   2.22E+00   3.5    5675.0  ! Tsang 1991
C3H4O-enone+OH=C3H3O-enone+H2O 4.00E+06   2.0      0.0   ! Marinov 1996
C3H4O-enone+O=C3H3O-enone+OH   7.60E+08   1.5   8500.0   ! Marinov 1996
C3H4O-enone+H=C3H3O-enone+H2   2.00E+05   2.5   2500.0   ! Marinov 1996
!C3H4O-enone+H=C2H5+CO      2.00E+13   0.0   2000.0   ! Marinov 1996
!C3H4O-enone+O=CH3+HCO+CO   3.00E+07   2.0      0.0   ! Marinov 1996
C3H4O+OH=C3H3O-enone+H2O 1.00E+13  0.0      0.0   ! Marinov 1996
C3H4O+O=C3H3O-enone+OH  7.24E+12   0.0   1970.0   ! Marinov 1996
!C3H4O+O=CH2CO+HCO+H 5.01E+07   1.76    76.0   ! Marinov 1996
C3H4O+H=C3H3O-enone+H2  3.98E+13   0.0   4200.0   ! Marinov 1996
!C3H4O+H=C2H4+HCO    2.00E+13   0.0   3500.0   ! Marinov 1996
!C3H4O+O2=C3H3O-enone+HO2 3.00E+13  0.0  36000.0   ! Marinov 1996
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C3H4O+O2=C3H3O-enone+HO2      3.01E+13    0.0   39.15E+03   !Based on
Baulch (1992) CH3CHO+O2=HO2+CH3CO
!C3H3O-enone=C2H3+CO        1.00E+14   0.0  34000.0   ! Marinov 1996
!C3H3O-enone+O=C2H3+CO2     1.00E+14   0.0      0.0   ! Marinov 1996
aC3H5+O2=C3H4O+OH   1.82E+13  -0.41 22859.0   ! Bozzelli 1993
!aC3H5+O2=aC3H4+HO2     4.99E+15  -1.4  22428.0   ! Bozzelli 1993
!The following two replaced by MRH C3H5O2 CBS-QB3 PES
!aC3H5+O2=CH2CHO+CH2O   1.06E+10  0.34  12838.0   ! Bozzelli 1993
!aC3H5+O2=C2H2+CH2O+OH  2.78E+25  -4.8  15468.0   ! Bozzelli 1993
!aC3H5+HO2=C3H5O-enal+OH    1.00E+13  0.0     0.0  !Tsang 1991
!C3H5O-enal+O2=C3H4O+HO2 4.00E+10  0.0  1100.0  ! Marinov 1998
!C3H5O-enal+CO=aC3H5+CO2    4.68E+2   3.16 5380.0  ! Marinov 1998
!C3H4O+H(+m)=C3H5O-enal(+m) 5.40E+11 0.454 2600. ! Marinov 1998
!   LOW/ 1.5e30 -4.8 5560./
!   TROE/0.78  94.  1555. 4200./
!  H2O/5./
!aC3H5+OH=aC3H4+H2O     1.00E+13  0.0       0.0   ! Tsang 1991
!aC3H5+H=aC3H4+H2       5.00E+13  0.0       0.0   ! Marinov 1996
!aC3H5+H=C3H6       1.88E+26  -3.6   5468.0   ! Marinov 1996
!aC3H5+O=C3H4O+H     1.81E+14  0.0       0.0   ! Slagle 1992
aC3H5+CH3=aC3H4+CH4    3.02E+12  -0.32  -131.0   ! Tsang 1991
pC3H5+O2=CH3CHO+HCO    1.09E+23  -3.29  3892.0   ! Marinov 1996
!pC3H5+O2=C3H4O-enone+H+O   1.60E+15  -0.78  3135.0   ! Marinov 1996
!pC3H5+O=C3H4O-enone+H      1.00E+14   0.0      0.0   ! Marinov 1996
!pC3H5+H=pC3H4+H2       2.00E+13   0.0      0.0   ! Marinov 1996
!pC3H5+OH=pC3H4+H2O     1.00E+13   0.0      0.0   ! Marinov 1996
!pC3H5+H=aC3H5+H        1.00E+14   0.0      0.0   ! Marinov 1996
!sC3H5+H=aC3H5+H        1.00E+14   0.0      0.0   ! Marinov 1996
sC3H5+O2=CH3CO+CH2O    1.09E+22  -3.29  3892.0   ! Marinov 1996
!sC3H5+O=CH2CO+CH3      1.00E+14   0.0      0.0   ! Marinov 1996
sC3H5+H=pC3H4+H2       4.00E+13   0.0      0.0   ! Marinov 1996
sC3H5+OH=pC3H4+H2O     2.00E+13   0.0      0.0   ! Marinov 1996
!aC3H4+H=pC3H3+H2      2.00E+7    2.0   5000.0   ! Marinov 1997
!aC3H4+O=C2H4+CO        1.34E+07   1.88   179.0   ! Marinov 1996
!aC3H4+OH=pC3H3+H2O    1.00E+7    2.0   1000.0   ! Marinov 1997
aC3H4+CH3=pC3H3+CH4   3.00E+01    3.5   5600.0   ! Marinov 1997
aC3H4=pC3H4            1.48E+13   0.0   60401.0  ! Marinov 1997
!pC3H4+H=pC3H3+H2      2.00E+7    2.0   5000.0   ! Marinov 1997
!pC3H4+O=C2H4+CO        1.50E+13   0.0   2102.0   ! Marinov 1996
!pC3H4+OH=pC3H3+H2O    1.00E+7    2.0   1000.0   ! Marinov 1997
!pC3H4+CH3=pC3H3+CH4   1.50E+0    3.5   5600.0   ! Marinov 1997
CH3+pC3H4=CH4+pC3H3     1.98E14     0.0   13.1e+03    !H_Abstraction
exact:      C/H3/Ct     C_methyl

!pC3H4+H=CH3+C2H2       5.12E+10   1.0   2060.0   ! Marinov 1997
! Reaction rate expression reported by Sharma et al. implemented; see
below
! Sharma, S.; Harper, M.R.; Green, W.H.,
!    "Modeling of 1,3-hexadiene, 2,4-hexadiene and 1,4-hexadiene doped
methane flames:
!    Flame modeling, Benzene and Styrene formation", Submitted to
Combust. Flame

!pC3H4+H(+m)=sC3H5(+m)  6.50E+12   0.0   2000.0   ! Wagner 1972
!   LOW / 8.45E+39  -7.27    6577.0 /               ! Marinov 1996
!aC3H4+H(+m)=aC3H5(+m)  1.20E+11   0.69  3007.0   ! Tsang 1992
!   LOW / 5.56E+33   -5.0    4448.0 /              ! Marinov 1996
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!aC3H4+H(+m)=sC3H5(+m)  8.49E+11   0.0   2000.0   ! Wagner 1972
!   LOW / 1.11E+34   -5.0    4448.0 /                ! Marinov 1996
! Estimate: This study divides the high pressure limit pre-exponential
factor by 10

!pC3H3+O2=CH2CO+HCO    3.00E+10   0.0   2868.0   ! Miller 1992
! D.K. Hahn, S.J. Klippenstein, J.A. Miller
! "A theoretical analysis of the reaction between propargyl and
molecular oxygen"
! Faraday Discuss. 119 (2001) 79-100
pC3H3+O2=CH2CO+HCO      1.7045e+05  1.7   1500.96

pC3H3+O=CH2O+C2H      1.40E+14   0.0      0.0   ! Pauwels 1995
!pC3H3+H=C3H2+H2       5.00e+13   0.0   1000.0   ! Pauwels 1995
!pC3H3+OH=C3H2+H2O     2.00E+13   0.0      0.0   ! Miller 1992
!pC3H3+CH3=C3H2+CH4    2.00E+13   0.0      0.0   ! Marinov 1997
!pC3H3+H(+m)=aC3H4(+m) 1.66E+15 -0.37      0.0   ! Marinov 1996
!   LOW / 3.36E+45 -8.52  6293.0  /           ! Kiefer 1995
!   H2O/5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ O2/2.0/ C2H2/2.0/
!pC3H3+H(+m)=pC3H4(+m) 1.66E+15 -0.37      0.0   ! Marinov 1996
!   LOW / 8.78E+45 -8.9   7974.0 /              ! Kiefer 1995
!   H2O /5.0/ H2/2.0/ CO2/3.0/ CO/2.0/ O2/2.0/ C2H2/2.0/
C3H2+O2=HCCO+CO+H      2.00E+12   0.0    1000.0  ! Pauwels 1995
!C3H2+O=C2H2+CO         1.00E+14   0.0       0.0  ! Pauwels 1995
C3H2+OH=C2H2+HCO       5.00E+13   0.0       0.0  ! Miller 1992



!RMG generated reactions and rate expressions

!!! H-abstraction of n-butanol
!nC4H10O+O=C4H9O-1+OH   9.540E+04   2.710 2106.00     !H_Abstraction
exact:      C/H3/Cs     O_atom_triplet
!nC4H10O+O=C4H9O-2+OH   4.289E+05   2.65  2583.65     !H_Abstraction
exact:      C/H2/NonDeC     O_atom_triplet
!nC4H10O+O=C4H9O-3+OH   4.289E+05   2.65  2583.65     !H_Abstraction
exact:      C/H2/NonDeC     O_atom_triplet
!nC4H10O+O=C4H9O-4+OH   4.289E+05   2.79  2183.65     !H_Abstraction
estimate: (Average:)    C/H2/CsO     O_atom_triplet
!nC4H10O+O=C4H9O-5+OH   1.000E+13   0.000 4690.00     !H_Abstraction
exact:      O/H/NonDeC     O_atom_triplet

!Values for -1,-4,-5 come from C2H5OH+O TST calculations:
!     C. W. Wu, Y. P. Lee, S. C. Xu, M. C. Lin, J. Phys. Chem. A 111
(2007) 6693-6703.
!Values for -2,-3 come from branching ratio for
k(nC4H10+O=OH+sC4H9)/k(nC4H10+O=OH+nC4H9):
!     N. Cohen, K. R. Westberg, J. Phys. Chem. Ref. Data 20 (1991) 1211-
1311.
! and k(nC4H10+O=OH+nC4H9) = 2*k(C2H5OH+O=OH+CH2CH2OH)
!     N. Cohen, K. R. Westberg, Int. J. Chem. Kinet. 18 (1986) 99-140.
nC4H10O+O=OH+C4H9O-1    9.7e2 3.23  4.66e+03
nC4H10O+O=OH+C4H9O-2    1.69e2      3.43  1.74e+03
nC4H10O+O=OH+C4H9O-3    1.69e2      3.43  1.74e+03
nC4H10O+O=OH+C4H9O-4    1.45e5      2.47  0.88e+03
nC4H10O+O=OH+C4H9O-5    1.46e-3     4.73  1.73e+03
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!!nC4H10O+H=C4H9O-1+H2  0.2E8       1.70  7680.0      !H_Abstraction
exact:      C/H3/Cs     H_rad
!nC4H10O+H=C4H9O-1+H2   1.040E+08   1.400 7510.00     !H_Abstraction
exact:      C/H3/Cs     H_rad
!!nC4H10O+H=C4H9O-2+H2  0.8E8       1.60  5980.0      !H_Abstraction
exact:      C/H2/NonDeC     H_rad
!!nC4H10O+H=C4H9O-3+H2  1.0E8       1.60  5980.0      !H_Abstraction
exact:      C/H2/NonDeC     H_rad
!!nC4H10O+H=C4H9O-4+H2  0.5E6       2.20  1530.0      !H_Abstraction
estimate: (Average:)    C/H2/CsO     H_rad
!!nC4H10O+H=C4H9O-5+H2  8.700E+08   1.390 10070.00    !H_Abstraction
exact:      O/H/NonDeC     H_rad

!CBS-QB3 calculations w/1DHR corrections
nC4H10O+H=H2+C4H9O-1    3.47e+06    2.27  7.88e+03
nC4H10O+H=H2+C4H9O-2    1.14e+06    2.25  5.44e+03
nC4H10O+H=H2+C4H9O-3    2.26e+06    2.15  5.66e+03
nC4H10O+H=H2+C4H9O-4    9.25e+05    2.28  3.76e+03
nC4H10O+H=H2+C4H9O-5    1.54e+05    2.48  8.92e+03

!nC4H10O+OH=H2O+C4H9O-1 0.90E+06    1.9   860.0 !H_Abstraction exact:
      C/H3/Cs     O_pri_rad
!nC4H10O+OH=H2O+C4H9O-1 0.30E+06    1.8   860.0       !H_Abstraction
exact:      C/H3/Cs     O_pri_rad
!nC4H10O+OH=H2O+C4H9O-2 1.90E+06    1.9   260.0       !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad
!nC4H10O+OH=H2O+C4H9O-3 3.90E+06    1.9   360.0       !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad
!nC4H10O+OH=H2O+C4H9O-4 3.90E+06    1.9   160.0       !H_Abstraction
estimate: (Average:)    C/H2/CsO     O_pri_rad
!nC4H10O+OH=H2O+C4H9O-5 2.46E+11    0.30  1834.0      !EtOH Marinov 1998
   ! Estimate: value for C2H5OH+OH=H2O+C2H5O, pre-exponential factor
divided by 3
!The following kinetics are from G3 PES of:
!     C.-W. Zhou, J. M. Simmie, H. J. Curran, Combust. Flame 158 (2011)
726-731
nC4H10O+OH=H2O+C4H9O-1  2.15e4      2.77  185.39
nC4H10O+OH=H2O+C4H9O-2  5.09e1      3.35  -4357.49
nC4H10O+OH=H2O+C4H9O-3  8.29e-1     3.74  -4073.35
nC4H10O+OH=H2O+C4H9O-4  4.56e3      2.81  -3685.89
nC4H10O+OH=H2O+C4H9O-5  5.88e2      2.82  -584.58

!!nC4H10O+CH3=C4H9O-1+CH4     0.400e+06   1.97  11230.0
      !H_Abstraction exact:   C/H3/Cs     C_methyl
!nC4H10O+CH3=C4H9O-1+CH4      0.440e+06   1.6   11050.0
      !H_Abstraction exact:   C/H3/Cs     C_methyl
!!nC4H10O+CH3=C4H9O-2+CH4     0.9900e+06  1.77  8230.0
      !H_Abstraction exact:   C/H2/NonDeC     C_methyl
!!nC4H10O+CH3=C4H9O-3+CH4     0.9900e+06  1.77  8230.0
      !H_Abstraction exact:   C/H2/NonDeC     C_methyl
!!nC4H10O+CH3=C4H9O-4+CH4     1.400e+06   1.82  6530.0
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_methyl
!!C4H9O-5+CH4=nC4H10O+CH3     1.20E-04    5.0   5580.0
      !H_Abstraction exact:   O_rad/NonDeC     C_methane
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!CBS-QB3 calculations w/1DHR corrections
nC4H10O+CH3=CH4+C4H9O-1 3.32e+01    3.38  9.88e+03
nC4H10O+CH3=CH4+C4H9O-2 9.29e+00    3.37  7.79e+03
nC4H10O+CH3=CH4+C4H9O-3 2.40e+01    3.24  8.06e+03
nC4H10O+CH3=CH4+C4H9O-4 1.53e+01    3.31  6.95e+03
nC4H10O+CH3=CH4+C4H9O-5 1.87e+00    3.50  6.00e+03

nC4H10O+CH2OH=C4H9O-1+CH3OH   0.540E+06   1.800 15050.00
      !H_Abstraction estimate: (Average:) C/H3/Cs     C_rad/H2/O
nC4H10O+CH2OH=C4H9O-2+CH3OH   0.99140E+06 1.753 12532.12
      !H_Abstraction estimate: (Average:) C/H2/NonDeC     C_rad/H2/O
nC4H10O+CH2OH=C4H9O-3+CH3OH   0.99140E+06 1.753 12532.12
      !H_Abstraction estimate: (Average:) C/H2/NonDeC     C_rad/H2/O
nC4H10O+CH2OH=C4H9O-4+CH3OH   0.99040E+06 1.786 13448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/O
nC4H10O+CH2OH=C4H9O-5+CH3OH   0.250E-04   5.000 12580.00
      !H_Abstraction estimate: (Average:) O/H/NonDeC     C_rad/H2/O

nC4H10O+CH3O=C4H9O-1+CH3OH    1.420E+11   0.000 7000.00
      !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
nC4H10O+CH3O=C4H9O-2+CH3OH    2.200E+11   0.000 4570.00
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
nC4H10O+CH3O=C4H9O-3+CH3OH    2.200E+11   0.000 4570.00
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
nC4H10O+CH3O=C4H9O-4+CH3OH    3.173E9     0.95  5644.0
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_rad/NonDeC
C4H9O-5+CH3OH=nC4H10O+CH3O    1.730E+01   3.400 -1140.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeC

nC4H10O+C2H5=C4H9O-1+C2H6     1.040E+05   1.900 11050.00
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
nC4H10O+C2H5=C4H9O-2+C2H6     0.2100E+06  1.670 8530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C2H5=C4H9O-3+C2H6     0.2100E+06  1.670 8530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C2H5=C4H9O-4+C2H6     2.040E+05   1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9O-5+C2H6=nC4H10O+C2H5     2.844e+12   0.0   9000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

nC4H10O+C3H7-1=C4H9O-1+C3H8   1.340E+05   1.900 12050.00
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
nC4H10O+C3H7-1=C4H9O-2+C3H8   5.040E+05   1.770 10530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C3H7-1=C4H9O-3+C3H8   5.040E+05   1.770 10530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C3H7-1=C4H9O-4+C3H8   5.040E+05   1.770 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
nC4H10O+C3H7-1=C4H9O-5+C3H8   7.550E-05   4.000 5580.00
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H9O-1+nC4H10=nC4H10O+C4H9-1 659.0       2.61  12920.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
nC4H10O+C4H9-1=C4H9O-2+nC4H10 3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C4H9-1=C4H9O-3+nC4H10 3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
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nC4H10O+C4H9-1=C4H9O-4+nC4H10 3.04E+06    1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9O-5+nC4H10=nC4H10O+C4H9-1 4.74E11     0.0   7000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H9O-1+nC4H10=nC4H10O+C4H9-2 1540.0      2.66  12100.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H2/NonDeC
C4H9O-2+nC4H10=nC4H10O+C4H9-2 15.2        3.19  10310.0
      !H_Abstraction exact:   C_rad/H/NonDeC     C/H2/NonDeC
C4H9O-3+nC4H10=nC4H10O+C4H9-2 15.2        3.19  10310.0
      !H_Abstraction exact:   C_rad/H/NonDeC     C/H2/NonDeC
nC4H10O+C4H9-2=C4H9O-4+nC4H10 3.04E06     1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H/NonDeC
C4H9O-5+nC4H10=nC4H10O+C4H9-2 7.25E10     0.0   4570.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H2/NonDeC

!HO2+C4H9O-1=O2+nC4H10O 3.00E+11    0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
!HO2+C4H9O-2=O2+nC4H10O 3.00E+11    0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/NonDeC
!HO2+C4H9O-3=O2+nC4H10O 3.00E+11    0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/NonDeC
!HO2+C4H9O-4=O2+nC4H10O 3.00E+11    0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/NonDeC
!HO2+C4H9O-5=O2+nC4H10O 1.75E+10    0.0   -3275.0
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/NonDeC

!C4H9O-1+H2O2=nC4H10O+HO2     1486.7      2.386 9690.0
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     O/H/NonDeO
!C4H9O-2+H2O2=nC4H10O+HO2     1486.7      2.386 9690.0
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     O/H/NonDeO
!C4H9O-3+H2O2=nC4H10O+HO2     1486.7      2.386 9690.0
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     O/H/NonDeO
!C4H9O-4+H2O2=nC4H10O+HO2     1486.7      2.386 9690.0
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     O/H/NonDeO
C4H9O-5+H2O2=nC4H10O+HO2      17.3        3.4   -1140.0
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeO

nC4H10O+C2H5O-1=C4H9O-1+C2H5OH      1077.0      2.71  13920.0
      !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
nC4H10O+C2H5O-1=C4H9O-2+C2H5OH      3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C2H5O-1=C4H9O-3+C2H5OH      3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
nC4H10O+C2H5O-1=C4H9O-4+C2H5OH      3.04E+06    1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9O-5+C2H5OH=nC4H10O+C2H5O-1      4.74E11     0.0   7000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H7-14+nC4H10O=C4H8-1+C4H9O-2      3.080E+03   2.660 10100.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C4H7-14+nC4H10O=C4H8-1+C4H9O-3      3.080E+03   2.660 10100.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
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C4H7-14+nC4H10O=C4H8-1+C4H9O-4      3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H8-1+C4H9O-5=C4H7-14+nC4H10O      1.420E+12   0.000 7000.00
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H8-1+C4H9O-2=C4H7-24+nC4H10O      1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H8-1+C4H9O-3=C4H7-24+nC4H10O      1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H8-1+C4H9O-4=C4H7-24+nC4H10O      1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H2/OneDeC
C4H8-1+C4H9O-5=C4H7-24+nC4H10O      1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/OneDeC

C4H6-1+C4H9O-1=C4H5-113+nC4H10O     3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H2/OneDeC
C4H6-1+C4H9O-2=C4H5-113+nC4H10O     3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H6-1+C4H9O-3=C4H5-113+nC4H10O     3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H6-1+C4H9O-4=C4H5-113+nC4H10O     3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H2/OneDeC
C4H6-1+C4H9O-5=C4H5-113+nC4H10O     1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/OneDeC

C4H6-12+C4H9O-5=C4H5-113+nC4H10O    1.030E+13   0.000 5940.00
      !H_Abstraction estimate: (Average:) Cd_pri     O_rad/NonDeC
C4H9O-5+C4H6-12=nC4H10O+iC4H5       7.460E+07   1.700 3643.88
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_rad/NonDeC
C2H3O-1+nC4H10O=C2H4O+C4H9O-1       1.510E+13   0.000 9175.00
      !H_Abstraction estimate: (Average:) Cd_pri_rad     C/H3/Cs
C2H3O-2+nC4H10O=C2H4O+C4H9O-1       1.510E+13   0.000 9175.00
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeO     C/H3/Cs

!!! Assisted C4H9O isomerization
nC4H10O+C4H9O-1=C4H9O-2+nC4H10O     3080.0      2.66        10100.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H2/NonDeC
nC4H10O+C4H9O-1=C4H9O-3+nC4H10O     3080.0      2.66        10100.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H2/NonDeC
nC4H10O+C4H9O-1=C4H9O-4+nC4H10O     3039788.2   1.8858      9448.34
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9O-5+nC4H10O=nC4H10O+C4H9O-1     1.422E12    0.0         7000.0
      !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
C4H9O-3+nC4H10O=nC4H10O+C4H9O-2     30.4        3.19        10310.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H/NonDeC
nC4H10O+C4H9O-2=C4H9O-4+nC4H10O     3039788.2   1.8858      9448.34
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H/NonDeC
C4H9O-5+nC4H10O=nC4H10O+C4H9O-2     1.45E11     0.0         4570.0
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
nC4H10O+C4H9O-3=C4H9O-4+nC4H10O     3039788.2   1.8858      9448.34
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H/NonDeC
C4H9O-5+nC4H10O=nC4H10O+C4H9O-3     1.45E11     0.0         4570.0
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
C4H9O-5+nC4H10O=nC4H10O+C4H9O-4     3.1729E9    0.95        5644.0
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/CsO

!!! H-abstraction of C4H8O-enol2
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C4H8O-enol2+CH3=C4H7O-13+CH4        2.410E+02   2.920 7160.00
      !H_Abstraction exact:   C/H3/Cd     C_methyl
C4H8O-enol2+H=C4H7O-13+H2           1.300E+06   2.380 2800.00
      !H_Abstraction exact:   C/H3/Cd     H_rad
!C4H8O-enol2+OH=C4H7O-13+H2O        7.460E+07   1.700 3643.88
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
C4H8O-enol2+OH=C4H7O-13+H2O         3.12E+06    2.0   298.757
      !Estimated based on C3H6+OH=H2O+aC3H5
C4H8O-enol2+CH3O=C4H7O-13+CH3OH     7.460E+07   1.700 3643.88
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_rad/NonDeC

!!! H-abstraction of C4H8O-enol3
C4H8O-enol3+CH3=C4H7O-13+CH4        5.460E+13   0.000 10400.00
      !H_Abstraction exact:   C/H2/OneDeC     C_methyl
C4H8O-enol3+H=C4H7O-13+H2           1.400E+06   2.360 1110.00
      !H_Abstraction exact:   C/H2/OneDeC     H_rad
C4H8O-enol3+CH2OH=C4H7O-13+CH3OH    3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     C_rad/H2/O
!C4H8O-enol3+OH=C4H7O-13+H2O        1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_pri_rad
C4H8O-enol3+OH=C4H7O-13+H2O         3.12E+06    2.0   298.757
      !Estimated based on C3H6+OH=H2O+aC3H5
C4H8O-enol3+CH3O=C4H7O-13+CH3OH     1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_rad/NonDeC

!!! Bond fissions of C4H8O-enol2 and C4H8O-enol3
!C4H7O-13+H=C4H8O-enol3              5.000E+13   0.000       0.00
      !R_Recombination estimate: (Average:)     C_rad/H/OneDeC     H_rad
!CH2OH+aC3H5=C4H8O-enol3                    1.150E+13   0.000       0.00
      !R_Recombination estimate: (Average:)     C_rad/H2/Cd
C_rad/H2/O
!C4H7-14+OH=C4H8O-enol3             7.690E+13   0.000       0.00
      !R_Recombination exact:       C_rad/H2/Cs     O_pri_rad
!C4H7-24+OH=C4H8O-enol2             1.500E+13   -0.150      291.67
      !R_Recombination estimate: (Average:)     C_rad/H2/Cd
O_pri_rad
!C4H7O-13+H=C4H8O-enol2             5.000E+13   0.000       0.00
      !R_Recombination estimate: (Average:)     C_rad/H2/Cd     H_rad

!!! H-abstractions of C4H8-1
!C4H8-1+CH3=C4H7-24+CH4       2.50e+11    0.0   8327.0
   ! Reaction rate expression from: Warnatz, J.; "Rate coefficients in
the C/H/O system" chapter in "Combustion Chemistry"
   !    ed. W.C. Gardiner, Jr., Springer-Verlag, NY 1984
!C4H8-1+H=C4H7-24+H2          4.400E+12   0.000 2110.00
      !H_Abstraction exact:   C/H2/OneDeC     H_rad
C4H8-1+CH3O=C4H7-24+CH3OH    1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_rad/NonDeC
C4H8-1+CH3=C4H7-14+CH4       8.340E+05   1.900 11050.00
      !H_Abstraction exact:   C/H3/Cs     C_methyl
C4H8-1+H=C4H7-14+H2          1.880E+08   1.750 7510.00
      !H_Abstraction exact:   C_rad/H2/Cs     H2
C4H8-1+OH=C4H7-14+H2O        3.890E+07   1.500 278.00
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
C4H8-1+CH3O=C4H7-14+CH3OH    1.420E+14   0.000 7000.00
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
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!!! H-abstractions of nC4H10
nC4H10+OH=C4H9-1+H2O    3.310E+07   1.800 950.00      !H_Abstraction
exact:      C/H3/Cs     O_pri_rad
nC4H10+OH=C4H9-2+H2O    5.360E+06   2.000 -590.00     !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad
nC4H10+CH3=C4H9-1+CH4   1.670E+06   1.900 11050.00    !H_Abstraction
exact:      C/H3/Cs     C_methyl
nC4H10+CH3=C4H9-2+CH4   5.800E+06   1.770 8530.00     !H_Abstraction
exact:      C/H2/NonDeC     C_methyl
nC4H10+H=C4H9-1+H2      3.770E+08   1.750 7510.00     !H_Abstraction
exact:      C/H3/Cs     H_rad
nC4H10+H=C4H9-2+H2      5.200E+08   1.690 4780.00     !H_Abstraction
exact:      C/H2/NonDeC     H_rad

!!! H-abstractions of C4H6-12
C4H6-12+H=C4H5-113+H2         5.060E+07   1.980 11780.00
      !H_Abstraction exact:   Cd_pri     H_rad
C4H6-12+CH3O=C4H5-113+CH3OH   1.030E+13   0.000 5940.00
      !H_Abstraction estimate: (Average:) Cd_pri     O_rad/NonDeC
CH3+C4H6-12=CH4+iC4H5         2.410E+02   2.920 7160.00
      !H_Abstraction exact:   C/H3/Cd     C_methyl
CH3O+C4H6-12=CH3OH+iC4H5      7.460E+07   1.700 3643.88
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_rad/NonDeC

!!! H-abstractions of C4H6-1
C4H6-1+CH3O=C4H5-113+CH3OH    1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_rad/NonDeC

!!! H-abstractions of C2H4O
C2H3O-1+CH4=C2H4O+CH3   6.360E+14   0.000 13700.00    !H_Abstraction
exact:      Cd_pri_rad      C_methane
C2H3O-1+H2=C2H4O+H      8.980E+12   0.000 10300.00    !H_Abstraction
exact:      Cd_pri_rad      H2
C2H4O+OH=C2H3O-2+H2O    1.110E+06   2.000 1450.00     !H_Abstraction
estimate: (Average:)    Cd/H/NonDeO     O_pri_rad
C2H3O-2+CH4=C2H4O+CH3   6.360E+14   0.000 13700.00    !H_Abstraction
estimate: (Average:)    Cd_rad/NonDeO     C_methane

CH3CHO+C2H5=CH3CO+C2H6  1.80E11     0.0   10210.0     !H_Abstraction
estimate: (Average:)    CO/H/NonDe      C_rad/H2/Cs

!!! Bond fissions
!C2H5+C2H5=nC4H10              3.150E+13   0.000       0.00
      !R_Recombination exact:       C_rad/H2/Cs     C_rad/H2/Cs
!CH3+C3H7-1=nC4H10                  3.370E+13   0.000       0.00
      !R_Recombination exact:       C_methyl      C_rad/H2/Cs
!CO+C2H4=C3H4O                 1.620E+08   1.701       82775.00
      !1,2_Insertion estimate: (Average:) Cd_pri     CO_birad
!HCO+C2H3=C3H4O                1.810E+13   0.000       0.00
      !R_Recombination exact:       Cd_pri_rad      CO_pri_rad
!CH3+pC3H3=C4H6-1              2.490E+16   -0.900      250.00
      !R_Recombination estimate: (Average:)     C_rad/H2/Ct     C_methyl
!C4H5-113+H=C4H6-1                  5.000E+13   0.000       0.00
      !R_Recombination estimate: (Average:)     C_rad/H/OneDeC     H_rad
!CH3+C3H2=C4H5-113                  1.446e+12   0.00000     0.00000
      !R_Recombination exact:       Cd_pri_rad      C_methyl
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!CH3+C3H5O-enol2=C4H8O-enol   2.490E+15   -0.900      250.00
      !R_Recombination estimate: (Average:)     C_methyl     C_rad/H2/Cd
!C2H5+C2H3O-1=C4H8O-enol            2.490E+15   -0.900      250.00
      !R_Recombination estimate: (Average:)     C_rad/H2/Cs
Cd_pri_rad
!H+iC4H5=C4H6-12              5.000E+13   0.000       0.00
      !R_Recombination estimate: (Average:)     C_rad/H2/Cd     H_rad
!CH3+HCO=CH3CHO               1.000E+13   0.000       0.00
      !R_Recombination exact:       C_methyl     CO_pri_rad
!CH3+HCO=CH3CHO               1.8E+13     0.0         0.00        !Tsang
review (1986)
!!! Beta-scissions
!C2H4+C2H5O-1=C4H9O-1   3.980E+03   2.440 5370.00
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H2     C_rad/H2/Cs
!C4H8O-enol3+H=C4H9O-1  1.300E+13   0.000 3260.00
      !R_Addition_MultipleBond exact:     Cd/H/Nd_Cd/H2     H_rad
!C4H8O-enol3+H=C4H9O-2  1.300E+13   0.000 3560.00
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/Nd     H_rad
!C4H8O-enol2+H=C4H9O-2  1.000E+13   0.000 3900.00
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/H/Nd
H_rad
!nC4H8O+H=C4H9O-5       1.000E+11   0.000 11900.00
      !R_Addition_MultipleBond estimate: (Average:)   CO/H/Nd_O
H_rad
!C3H7-1+CH2O=C4H9O-5    7.940E+10   0.000 6700.00
      !R_Addition_MultipleBond exact:     C_rad/H2/Cs     CO/H2_O
!C3H4O+H=C3H5O-enol2    2.260E+12   0.147 2532.84
      !R_Addition_MultipleBond estimate: (Average:)   OCO     H_rad
C2H2+C2H3=nC4H5         2.510E+05   1.900 2110.00
      !R_Addition_MultipleBond exact:     Ct/H_Ct/H     Cd_pri_rad
!C4H4+H=C4H5-113        3.710E+12   0.000 1000.00
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/De     H_rad
HCCOH+H=C2H3O-2         1.120E+14   0.000 3700.00
      !R_Addition_MultipleBond exact:     Ct/H_Ct/Nd     H_rad
HCCOH+H=C2H3O-1         5.770E+13   0.000 5300.00
      !R_Addition_MultipleBond exact:     Ct/Nd_Ct/H     H_rad
C2H2+OH=C2H3O-1         1.210E+12   0.000 460.00
      !R_Addition_MultipleBond exact:     Ct/H_Ct/H     O_pri_rad
!C4H6-12+H=C4H7-24            2.560E+13   0.000 3700.00
      !R_Addition_MultipleBond exact:     Ca_Cd/H/Nd     H_rad

!!! Isomerizations
!C4H7-14=C4H7-24        2.820E+08   1.280 27900.00    !intra_H_migration
exact:      Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe

!!! Reaction rate expressions from Leeds mechanism
   ! http://www.chem.leeds.ac.uk/Combustion/mechanisms/metan15.dat
C2H4+CH2(S)=C3H6              9.640E+13   0.000 0.00
!C4H2+OH=C3H2+HCO             10.0E+12    0.000 -410.00
   ! Pre-exponential factor was multiplied by 1.5 (stated uncertainty is
1.5)
C4H2+O=C3H2+CO                7.890E+12   0.000 1350.00

!!! Reaction rate expressions from:
   ! Wang, H.; Frenklach, M.; "A Detailed Kinetic Modeling Study of
Aromatics Formation in Laminar Premixed
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   !    Acetylene and Ethylene Flames", Combust. Flame (1997) v.110 173-
221
!nC4H3=iC4H3                  4.100E+43   -9.490      53000.00    !Rxn
254, 760 torr
iC4H3+H=C2H2+C2H2       2.800E+23   -2.550      10780.00    !Rxn 257,
760 torr
iC4H3+H=C4H2+H2         3.000E+13   0.000       0.00        !Rxn 261
iC4H3+O2=HCCO+CH2CO     7.860E+16   -1.800      0.00        !Rxn 264
nC4H3+C2H2=C6H5         9.600E+70   -17.770     31300.00    !Rxn 267,
760 torr
nC4H3+C2H2=C6H4+H       6.900E+46   -10.010     30100.00    !Rxn 268,
760 torr
C4H4+O=pC3H4+CO         2.700E+13   0.000       1720.00     !Rxn 275
!C4H6-12+H=C4H6-13+H    2.000E+13   0.000       4000.00     !Rxn 296
C4H6-12+H=iC4H5+H2      1.700E+05   2.500       2490.00     !Rxn 297
C4H6-12+OH=iC4H5+H2O    3.100E+06   2.000       -298.00     !Rxn 301

!!! Reaction rate expression from:
   ! Lindstedt, R.P.; Skevis, G., "Benzene formation chemistry in
premixed 1,3-butadiene flames",
   !    Symp. Int. Combust. Proc. (1996) v.26 703-709
!C4H6-13+OH=nC4H5+H2O   2.000E+07   2.000 5000.00
!C4H6-13+OH=iC4H5+H2O   1.000E+07   2.000 2000.00
   ! Estimate, based on C4H6-13+OH=nC4H5+H2O: Decreased pre-exponential
factor by 2,
   !    decreased activation energy by 3 kcal/mol
!H+C4H6-13=aC3H4+CH3    3.000E+13   0.000 8100.00
!H+C4H6-12=aC3H4+CH3    6.000E+13   0.000 2100.00

!C2H2+C2H=C4H2+H  1.030E+13   0.000 0.00
   ! Tsang, W.; Hampson, R.F., "Chemical kinetic database for combustion
chemistry.  Part I.
   !    Methane and related compounds", J. Phys. Chem. Ref. Data, (1986)
v.15 1087-1279
   !    Discussion on p.1224, Entry (21,20)

nC4H3(+M)=C4H2+H(+M)    7.500E+13   0.000 39000.00    ! Miller 1992
   LOW / 1.000E+14      0.000 30000.00 /              ! Miller 1992
iC4H3(+M)=C4H2+H(+M)    7.500E+13   0.000 50000.00    ! Marinov 1998
   LOW / 2.000E+15      0.000 40000.00 /              ! Marinov 1998
nC4H5(+m)=C4H4+H(+m)    1.00E+14    0.0   37000.0     ! Miller 1992
   LOW / 1.00E+14       0.0   30000.0 /               ! Miller 1992

!!! Enol-Aldehyde tautomerization
!C2H4O=CH3CHO           8.59E+11    0.318 55900.00
!C4H8O-enol=nC4H8O            8.59E+11    0.318 55900.00
!C2H3O-1=CH2CHO         8.59E+11    0.318 55900.00
!C3H6O-enol=C3H6O       8.59E+11    0.318 55900.00
!H2CCCH3[OH]=acetone    8.59E+11    0.318 55900.00

!!! Reaction rate expressions from KVG
C4H4+H=nC4H3+H2         2.250E+14   0.000 18390.00
C2H5+C2H4=C2H3+C2H6     7.270E+05   2.000 9200.00     !
!C2H5+C2H4=C2H3+C2H6    6.33e+02    3.13  18004.3
CH3+C4H4=CH4+iC4H3      5.500E+11   0.000 14390.00
CH3+C4H4=CH4+nC4H3      1.440e+13   0.000 19140.00
C4H4+C2H3=benzene+H     1.900E+12   0.000 2509.00
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!!!! Reactions involving C3H6O, C3H5OJ(8), C3H5OJ(12), C3H5OJ(13)
!CO+C2H6=C3H6O                          5.4840000e+05     2.53000e+00
      8.55000e+04 !1,2_Insertion exact:   CO_birad     C_pri/NonDeC
!CO+C2H5=C3H5OJ(13)                     1.2125098e+08     1.70125e+00
      8.27750e+04 !1,2_Insertion exact:   CO_birad     R_H
C3H6O+C2H5=C3H5OJ(8)+C2H6               3.8000000e+11     0.00000e+00
      7.21000e+03 !H_Abstraction estimate:   CO/H/NonDe     C_rad/H2/Cs
C3H6O+C2H5=C3H5OJ(12)+C2H6              5.5637357e+02     2.82875e+00
      9.54750e+03 !H_Abstraction estimate:   C/H2/OneDeC     C_rad/H2/Cs
C3H5OJ(13)+C2H6=C3H6O+C2H5              3.9540000e+03     2.71000e+00
      1.29200e+04 !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
C3H5OJ(12)+C3H6O=C3H6O+C3H5OJ(8)        1.0533755e+08     1.14500e+00
      6.32500e+03 !H_Abstraction estimate:   C_rad/H/OneDeC
CO/H/NonDe
C3H5OJ(13)+C3H6O=C3H6O+C3H5OJ(8)        3.8000000e+11     0.00000e+00
      7.21000e+03 !H_Abstraction estimate:   C_rad/H2/Cs     CO/H/NonDe
C3H5OJ(13)+C3H6O=C3H6O+C3H5OJ(12)       5.5637357e+02     2.82875e+00
      9.54750e+03 !H_Abstraction estimate:   C_rad/H2/Cs     C/H2/OneDeC
!CO+C2H5=C3H5OJ(8)                              1.5100000e+11     0.00000e+00
      4.81000e+03 !R_Addition_COm exact:   COm     C_rad/H2/Cs
!HCO+C2H4=C3H5OJ(13)                    1.0400000e+12     0.00000e+00
      6.56000e+03 !R_Addition_MultipleBond estimate:   CO_pri_rad
Cd/H2_Cd/H2
!C3H4O+H=C3H5OJ(13)             8.8500000e+13     0.00000e+00 4.30000e+03
      !R_Addition_MultipleBond exact:   Cd/H/De_Cd/H2     H_rad
!HCO+C2H5=C3H6O                         1.8100000e+13     0.00000e+00
      0.00000e+00 !R_Recombination exact:   C_rad/H2/Cs     CO_pri_rad
!C3H5OJ(8)+H=C3H6O                              5.0000000e+13     0.00000e+00
      0.00000e+00 !R_Recombination estimate:   CO_rad/NonDe     H_rad
!C3H5OJ(12)+H=C3H6O                     5.0000000e+13     0.00000e+00
      0.00000e+00 !R_Recombination estimate:   C_rad/H/OneDeC     H_rad
!C3H5OJ(13)=C3H5OJ(8)                   2.0476980e+08     1.13807e+00
      3.48303e+04 !intra_H_migration estimate:   Others-R3H_SS
C_rad_out_2H     CO_H_out
!C3H5OJ(12)=C3H5OJ(8)                   2.0476980e+08     1.13807e+00
      3.48303e+04 !intra_H_migration estimate:   Others-R2H_S
C_rad_out_H/NonDeC     CO_H_out
!C3H5OJ(13)=C3H5OJ(12)                  2.8200000e+08     1.28000e+00
      2.79000e+04 !intra_H_migration exact:   Others-R2H_S
C_rad_out_2H     Cs_H_out_H/OneDe
C3H6O+H=C3H5OJ(8)+H2                    2.0700000e+07     1.76000e+00
      6.70000e+02 !H_Abstraction exact:   CO/H/NonDe     H_rad
C3H6O+H=C3H5OJ(12)+H2                   1.3980000e+06     2.36000e+00
      5.11000e+03 !H_Abstraction exact:   C/H2/OneDeC     H_rad
C3H6O+H=C3H5OJ(13)+H2                   1.8840000e+08     1.75000e+00
      7.51000e+03 !H_Abstraction exact:   C/H3/Cs     H_rad

!!! Reactions involving nC4H8O, C4H7OJ(8), C4H7OJ(12), C4H7OJ(13),
C4H7OJ(16)
nC4H8O+H=C4H7OJ(8)+H2                   2.0700000e+07     1.76000e+00
      6.70000e+02 !H_Abstraction exact:   CO/H/NonDe     H_rad
nC4H8O+H=C4H7OJ(12)+H2                  1.3980000e+06     2.06000e+00
      1.11000e+03 !H_Abstraction exact:   C/H2/OneDeC     H_rad
nC4H8O+H=C4H7OJ(13)+H2                  2.6000000e+08     1.69000e+00
      4.78000e+03 !H_Abstraction exact:   C/H2/NonDeC     H_rad
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nC4H8O+H=C4H7OJ(16)+H2              1.8840000e+08     1.75000e+00
      7.51000e+03 !H_Abstraction exact:   H_rad     C/H3/Cs
nC4H8O+CH3=C4H7OJ(8)+CH4                    2.9200000e+04     2.29000e+00
      5.44000e+03 !H_Abstraction exact:   CO/H/NonDe     C_methyl
nC4H8O+CH3=C4H7OJ(12)+CH4           4.0000000e+11     0.00000e+00
      9.50000e+03 !H_Abstraction estimate:   C/H2/OneDeC     C_methyl
nC4H8O+CH3=C4H7OJ(13)+CH4           2.9000000e+06     1.77000e+00
      8.53000e+03 !H_Abstraction exact:   C/H2/NonDeC     C_methyl
nC4H8O+CH3=C4H7OJ(16)+CH4           8.3400000e+05     1.90000e+00
      1.10500e+04 !H_Abstraction exact:   C_methyl     C/H3/Cs
!C3H5OJ(13)+CH3=nC4H8O              3.3700000e+13     0.00000e+00
      0.00000e+00 !R_Recombination exact:   C_rad/H2/Cs     C_methyl
!C4H7OJ(16)+H=nC4H8O                1.0000000e+14     0.00000e+00
      0.00000e+00 !R_Recombination exact:   C_rad/H2/Cs     H_rad
C4H7OJ(16)+nC4H8O=nC4H8O+C4H7OJ(8)  3.8000000e+11     0.00000e+00
      7.21000e+03 !H_Abstraction estimate:   C_rad/H2/Cs     CO/H/NonDe
C4H7OJ(16)+nC4H8O=nC4H8O+C4H7OJ(12) 5.5637357e+02     2.82875e+00
      9.54750e+03 !H_Abstraction estimate:   C_rad/H2/Cs     C/H2/OneDeC
C4H7OJ(16)+nC4H8O=nC4H8O+C4H7OJ(13) 3.0800000e+03     2.66000e+00
      1.01000e+04 !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C4H7OJ(12)+nC4H8O=nC4H8O+C4H7OJ(8)  1.0533755e+08     1.14500e+00
      6.32500e+03 !H_Abstraction estimate:   C_rad/H/OneDeC
CO/H/NonDe
C4H7OJ(13)+nC4H8O=nC4H8O+C4H7OJ(8)  1.0533755e+08     1.14500e+00
      6.32500e+03 !H_Abstraction estimate:   C_rad/H/NonDeC
CO/H/NonDe
nC4H8O+C4H7OJ(12)=C4H7OJ(13)+nC4H8O 3.0400000e+01     3.19000e+00
      1.03100e+04 !H_Abstraction estimate:   C/H2/NonDeC
C_rad/H/OneDeC
!C4H7OJ(12)=C4H7OJ(8)               2.0476980e+08     1.13807e+00
      3.48303e+04 !intra_H_migration estimate:   Others-R2H_S
C_rad_out_H/NonDeC     CO_H_out
!C4H7OJ(16)=C4H7OJ(12)              3.3200000e+08     1.10000e+00
      2.94000e+04 !intra_H_migration exact:   Others-R3H_SS
C_rad_out_2H     Cs_H_out_H/OneDe
!C4H7OJ(16)=C4H7OJ(13)              1.9380000e+10     8.90000e-01
      3.58000e+04 !intra_H_migration exact:   Others-R2H_S
C_rad_out_2H     Cs_H_out_H/NonDeC
!HCO+C3H6=C4H7OJ(13)                5.2000000e+11     0.00000e+00
      6.56000e+03 !R_Addition_MultipleBond estimate:   CO_pri_rad
Cd/H2_Cd/H/Nd
!CH2CHO+C2H4=C4H7OJ(16)             4.9654773e+10     2.44000e-01
      9.08750e+03 !R_Addition_MultipleBond estimate:   C_rad/H2/CO
Cd/H2_Cd/H2

!!! Reactions involving C4H7-14, C4H7-24, C4H7-22, and C4H7-12 (w/O2,
OH, HO2, and O)
O2+C4H7-14=HO2+C4H6-13        3.616E11    0.0         0.0
      !Disproportionation_O2d estimate: (Average:)    O2d
C/H2/De_Csrad
O2+C4H7-24=HO2+C4H6-13        7.56E11     0.0         0.0
      !Disproportionation_O2d exact:      O2d     Cmethyl_Csrad
O2+C4H7-24=HO2+C4H6-12        2.42E12     0.0         13550.00
      !Disproportionation_O2d exact:      O2d     Cdpri_Csrad
C4H7-14+HO2=C4H8-1+O2         3.000e11    0.0         0.0
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs     O_Orad
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```
C4H7-24+HO2=C4H8-1+O2         3.000e11    0.0         0.0
      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
O_Orad
HO2+C4H7-14=H2O2+C4H6-13      1.140E13    -0.071      -2.17
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/De_Csrad
HO2+C4H7-24=H2O2+C4H6-13      7.230E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
HO2+C4H7-24=H2O2+C4H6-12      6.030E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Csrad
OH+C4H7-14=H2O+C4H6-13        1.140E13    -0.071      -2.17
      !Disproportionation estimate: (Average:)  O_pri_rad
C/H2/De_Csrad
OH+C4H7-24=H2O+C4H6-12        6.03E12     0.0         0.0
      !Disproportionation exact:    O_pri_rad     Cdpri_Csrad
O+C4H7-14=OH+C4H6-13          3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/De_Csrad
O+C4H7-24=OH+C4H6-13          9.030E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
Cmethyl_Csrad
O+C4H7-24=OH+C4H6-12          7.226E12    -0.0498     -56.789
      !Disproportionation estimate: (Average:)  O_atom_triplet
Cdpri_Csrad
O2+C4H7-22=HO2+C4H6-12        7.560E11    0.0         0.0
      !Disproportionation_O2d estimate: (Average:)    O2d
Cmethyl_Cdrad
HO2+C4H7-22=H2O2+C4H6-12      5.115E13    -0.173      -1.806
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Cdrad
OH+C4H7-22=H2O+C4H6-12        5.115E13    -0.173      -1.806
      !Disproportionation estimate: (Average:)  O_pri_rad
Cmethyl_Cdrad
O+C4H7-22=OH+C4H6-12          9.030E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
Cmethyl_Cdrad
O2+C4H7-12=HO2+C4H6-12        3.616E11    0.0         0.0
      !Disproportionation_O2d estimate: (Average:)    O2d
C/H2/Nd_Cdrad
HO2+C4H7-12=H2O2+C4H6-12      4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Cdrad
OH+C4H7-12=H2O+C4H6-12        4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_pri_rad
C/H2/Nd_Cdrad
O+C4H7-12=OH+C4H6-12          3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/Nd_Cdrad

!!! Reactions involving C4H7-22, C4H7-12, C4H7-11
!C4H6-2+H=C4H7-22       5.004E13    0.0   4100.0
      !R_Addition_MultipleBond estimate: (Average:)   Ct/Nd_Ct/Nd
H_rad
!pC3H4+CH3=C4H7-22             1.32E14     0.0   10300.0
      !R_Addition_MultipleBond exact:     Ct/H_Ct/Nd     C_methyl
```

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!C4H6-12+H=C4H7-22            6.68E13     0.0   2900.0
      !R_Addition_MultipleBond exact:     Cd/H2_Ca     H_rad
!C4H7-22=C4H7-24        7.74E9      1.08  38700.0     !intra_H_migration
exact:      R3H_DS     Cd_rad_out_singleNd     Cs_H_out_2H
!     DUPLICATE
!C4H7-22=C4H7-24        7.32E9      1.12  41300.0     !intra_H_migration
exact:      Others-R2H_S    Cd_rad_out_double     Cs_H_out_2H
!     DUPLICATE
!C4H6-1+H=C4H7-12       1.12E14     0.0   3700.0
      !R_Addition_MultipleBond exact:     Ct/H_Ct/Nd     H_rad
!aC3H4+CH3=C4H7-12             9.23E12     0.0   9400.0
      !R_Addition_MultipleBond exact:     Cd/H2_Ca     C_methyl
!C4H6-12+H=C4H7-12             1.0E13      0.0   2900.0
      !R_Addition_MultipleBond exact:     Cd/H/Nd_Ca     H_rad
!C2H2+C2H5=C4H7-11             2.505E10    0.0   6990.0
      !R_Addition_MultipleBond exact:     Ct/H_Ct/H     C_rad/H2/Cs
!C4H6-1+H=C4H7-11       5.77E13     0.0   5300.0
      !R_Addition_MultipleBond exact:     Ct/Nd_Ct/H     H_rad
!C4H7-12=C4H7-24        1.448E10    0.82  37500.0     !intra_H_migration
estimate: (Average:)    Others-R2H_S    Cd_rad_out_double
Cs_H_out_H/NonDeC
!C4H7-11=C4H7-24        1.846E10    0.74  34700.0     !intra_H_migration
exact:      R3H_DS     Cd_rad_out_singleH     Cs_H_out_H/NonDeC
!C4H7-11=C4H7-14        6.143E8     1.138 34830.32    !intra_H_migration
estimate: (Average:)    R4H_DSS     Cd_rad_out_singleH     Cs_H_out_2H
!C4H7-12=C4H7-14        2.304E9     1.24  36300.0     !intra_H_migration
exact:      Others-R3H_SS    Cd_rad_out_double     Cs_H_out_2H
!C4H7-11=C4H7-12        3.24E11     0.73  42400.0     !intra_H_migration
exact:      R2H_D     Cd_rad_out_singleH     Cd_H_out_singleNd

!!! Disproportionation reactions
O2+C2H5O-1=HO2+C2H4O                3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
HO2+C2H5O-1=H2O2+C2H4O              4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
O+C2H5O-1=OH+C2H4O                  3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/Nd_Csrad

O2+C4H9-1=HO2+C4H8-1                3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
!OH+C4H9-1=H2O+C4H8-1               4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad
HO2+C4H9-1=H2O2+C4H8-1              4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
!O+C4H9-1=OH+C4H8-1                 3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/Nd_Csrad

HO2+C2H5=H2O2+C2H4                  7.230E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
O+C2H5=OH+C2H4                      9.030E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
Cmethyl_Csrad
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HO2+C3H7-1=H2O2+C3H6                4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
O+C3H7-1=OH+C3H6                    3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/Nd_Csrad

HO2+CH2OH=H2O2+CH2O                 1.21E13     0.0         0.0
      !Disproportionation exact:    O_rad/NonDeO     O_Csrad

O2+C4H9O-4=HO2+C4H8O-enol           3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
!O2+C4H9O-4=HO2+nC4H8O              2.28E12     0.0         0.0
      !Disproportionation_O2d exact:      O2d     O_Csrad
O2+C4H9O-5=HO2+nC4H8O               3.616E11    0.0         0.0
      !Disproportionation_O2d estimate: (Average:)    O2d
C/H2/Nd_Orad
!HO2+C4H9O-4=H2O2+C4H8O-enol        4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
HO2+C4H9O-4=H2O2+C4H8O-enol         3.01E11     0.0   0.0   !Based on
C2H5+HO2=H2O2+C2H4 [Tsang and Hampson, J. Phys. Chem. Ref. Data. 15
(1986)]
HO2+C4H9O-4=H2O2+nC4H8O             1.21E13     0.0         0.0
      !Disproportionation exact:    O_rad/NonDeO     O_Csrad
HO2+C4H9O-5=H2O2+nC4H8O             4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Orad
!OH+C4H9O-4=H2O+C4H8O-enol          4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad
OH+C4H9O-4=H2O+nC4H8O               2.41E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     O_Csrad
O+C4H9O-5=OH+nC4H8O                 3.620E12    0.0         0.0
      !Disproportionation estimate: (Average:)  O_atom_triplet
C/H2/Nd_Orad

CH3+C4H9O-4=CH4+C4H8O-enol          2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad
CH3+C4H9O-4=CH4+nC4H8O              2.41E12     0.0         0.0
      !Disproportionation exact:    C_methyl     O_Csrad
CH3+C4H9O-5=CH4+nC4H8O              3.783E13    -0.355      -10.834
      !Disproportionation estimate: (Average:)  C_methyl
C/H2/Nd_Orad
C2H5+C4H9O-4=C2H6+C4H8O-enol        2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C2H5+C4H9O-4=C2H6+nC4H8O                  2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad
C2H5+C4H9O-5=C2H6+nC4H8O                  3.783E13    -0.355      -
10.834      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/Nd_Orad

C2H5+CH2OH=C2H6+CH2O                2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad
CH3+CH2OH=CH4+CH2O                  2.41E12     0.0         0.0
      !Disproportionation exact:    C_methyl     O_Csrad
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C2H5+C3H7-1=C2H6+C3H6               2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
CH3+C3H7-1=CH4+C3H6                 2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad

C2H5+C2H5=C2H6+C2H4                 6.9E13      -0.35       0.0
      !Disproportionation exact:    C_rad/H2/Cs     Cmethyl_Csrad
CH3+C2H5=CH4+C2H4                   2.823E11    0.68        0.0
      !Disproportionation exact:    C_methyl     Cmethyl_Csrad

C2H5+C2H5O-1=C2H6+C2H4O             2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
CH3+C2H5O-1=CH4+C2H4O               2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad

C2H5+C4H9-1=C2H6+C4H8-1             2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
CH3+C4H9-1=CH4+C4H8-1               2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad

CH2OH+CH2OH=CH3OH+CH2O              4.82E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     O_Csrad
CH3O+CH2OH=CH3OH+CH2O               2.41E13     0.0         0.0
      !Disproportionation exact:    O_rad/NonDeC     O_Csrad
C2H5O-1+CH2OH=C2H5OH+CH2O           2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad
C4H9-1+CH2OH=nC4H10+CH2O            2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad

CH2OH+C2H5O-1=CH3OH+C2H4O           9.64E11     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     C/H2/Nd_Csrad
CH3O+C2H5O-1=CH3OH+C2H4O            4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Csrad
C2H5O-1+C2H5O-1=C2H5OH+C2H4O        2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C4H9-1+C2H5O-1=nC4H10+C2H4O         2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad

CH2OH+C4H9-1=CH3OH+C4H8-1           9.64E11     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     C/H2/Nd_Csrad
CH3O+C4H9-1=CH3OH+C4H8-1            4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Csrad
C2H5O-1+C4H9-1=C2H5OH+C4H8-1        2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C4H9-1+C4H9-1=nC4H10+C4H8-1         2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad

CH3O+C2H5=CH3OH+C2H4                7.230E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
Cmethyl_Csrad
C4H9-1+C2H5=nC4H10+C2H4             6.9E13      -0.35       0.0
      !Disproportionation exact:    C_rad/H2/Cs     Cmethyl_Csrad

CH2OH+C3H7-1=CH3OH+C3H6             9.64E11     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     C/H2/Nd_Csrad
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CH3O+C3H7-1=CH3OH+C3H6              4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Csrad
C2H5O-1+C3H7-1=C2H5OH+C3H6          2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C4H9-1+C3H7-1=nC4H10+C3H6           2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad

CH2OH+C4H9O-4=CH3OH+C4H8O-enol      9.64E11     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     C/H2/Nd_Csrad
CH2OH+C4H9O-4=CH3OH+nC4H8O          4.82E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/O     O_Csrad
CH3O+C4H9O-4=CH3OH+C4H8O-enol       4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Csrad
CH3O+C4H9O-4=CH3OH+nC4H8O           2.41E13     0.0         0.0
      !Disproportionation exact:    O_rad/NonDeC     O_Csrad
C2H5O-1+C4H9O-4=C2H5OH+C4H8O-enol   2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C2H5O-1+C4H9O-4=C2H5OH+nC4H8O       2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad
C4H9-1+C4H9O-4=nC4H10+C4H8O-enol    2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C4H9-1+C4H9O-4=nC4H10+nC4H8O        2.41E12     0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     O_Csrad

CH2OH+C4H9O-5=CH3OH+nC4H8O          3.783E13    -0.355      -10.834
      !Disproportionation estimate: (Average:)  C_rad/H2/O
C/H2/Nd_Orad
CH3O+C4H9O-5=CH3OH+nC4H8O           4.820E13    0.0         0.0
      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Orad
C2H5O-1+C4H9O-5=C2H5OH+nC4H8O       3.783E13    -0.355      -10.834
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/Nd_Orad
C4H9-1+C4H9O-5=nC4H10+nC4H8O        3.783E13    -0.355      -10.834
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/Nd_Orad

C2H5+C4H7-12=C2H6+C4H6-12           3.783E13    -0.355      -10.834
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/Nd_Cdrad
C2H5+C4H7-22=C2H6+C4H6-12           5.115E13    -0.173      -1.806
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
Cmethyl_Cdrad
CH3+C4H7-22=CH4+C4H6-12             5.115E13    -0.1730     -1.806
      !Disproportionation estimate: (Average:)  C_methyl
Cmethyl_Cdrad
C2H5+C4H7-24=C2H6+C4H6-12           9.64E11     0.0         -130.0
      !Disproportionation exact:    C_rad/H2/Cs     Cdpri_Csrad
C2H5+C4H7-24=C2H6+C4H6-13           6.9E13      -0.35       0.0
      !Disproportionation exact:    Cmethyl_Csrad     C_rad/H2/Cs
C2H5+C4H7-14=C2H6+C4H6-13           1.140E13    -0.071      -2.167
      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/De_Csrad
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CH3+C4H7-14=CH4+C4H6-13             1.140E13    -0.071      -2.167
      !Disproportionation estimate: (Average:)  C_methyl
C/H2/De_Csrad

H+C2H5O-1=H2+C2H4O                  3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
H+C4H9-1=H2+C4H8-1                  3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
H+C3H7-1=H2+C3H6                    3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
H+C4H9O-4=H2+C4H8O-enol             3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
H+C4H9O-4=H2+nC4H8O                 6.03E12     0.0         0.0
      !Disproportionation exact:    H_rad     O_Csrad
H+C4H9O-5=H2+nC4H8O                 3.62E12     0.0         0.0
      !Disproportionation estimate: (Average:)  H_rad     C/H2/Nd_Orad

O2+C4H9O-1=HO2+C4H8O-enol3          3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
O2+C4H9O-2=HO2+C4H8O-enol3          7.56E11     0.0         0.0
      !Disproportionation_O2d exact:      O2d     Cmethyl_Csrad
O2+C4H9O-2=HO2+C4H8O-enol2          3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
O2+C4H9O-3=HO2+C4H8O-enol2          3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad
O2+C4H9O-3=HO2+C4H8O-enol           3.616E11    0.0         0.0
      !Disproportionation_O2d exact:      O2d     C/H2/Nd_Csrad

!OH+C4H9O-1=H2O+C4H8O-enol3         4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad
!OH+C4H9O-2=H2O+C4H8O-enol3         7.23E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     Cmethyl_Csrad
!OH+C4H9O-2=H2O+C4H8O-enol2         4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad
!OH+C4H9O-3=H2O+C4H8O-enol2         4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad
!OH+C4H9O-3=H2O+C4H8O-enol          4.82E13     0.0         0.0
      !Disproportionation exact:    O_pri_rad     C/H2/Nd_Csrad

H+C4H9O-1=H2+C4H8O-enol3            3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
CH3+C4H9O-1=CH4+C4H8O-enol3         2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad
C2H5+C4H9O-1=C2H6+C4H8O-enol3       2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
H+C4H9O-2=H2+C4H8O-enol3            1.083E13    0.0         0.0
      !Disproportionation exact:    H_rad     Cmethyl_Csrad
H+C4H9O-2=H2+C4H8O-enol2            3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
CH3+C4H9O-2=CH4+C4H8O-enol3         2.823E11    0.68        0.0
      !Disproportionation exact:    C_methyl     Cmethyl_Csrad
CH3+C4H9O-2=CH4+C4H8O-enol2         2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad
C2H5+C4H9O-2=C2H6+C4H8O-enol3       6.9E13      -0.35       0.0
      !Disproportionation exact:    C_rad/H2/Cs     Cmethyl_Csrad
C2H5+C4H9O-2=C2H6+C4H8O-enol2       2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
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H+C4H9O-3=H2+C4H8O-enol2            3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
H+C4H9O-3=H2+C4H8O-enol             3.62E12     0.0         0.0
      !Disproportionation exact:    H_rad     C/H2/Nd_Csrad
CH3+C4H9O-3=CH4+C4H8O-enol2         2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad
CH3+C4H9O-3=CH4+C4H8O-enol          2.3E13      -0.32       0.0
      !Disproportionation exact:    C_methyl     C/H2/Nd_Csrad
C2H5+C4H9O-3=C2H6+C4H8O-enol2       2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad
C2H5+C4H9O-3=C2H6+C4H8O-enol        2.9E12      0.0         0.0
      !Disproportionation exact:    C_rad/H2/Cs     C/H2/Nd_Csrad

!!! H-abstraction of C4H8-1
C4H7-11+H2=C4H8-1+H     4.49E12     0.0   10300.0     !H_Abstraction
exact:      Cd_pri_rad     H2
C4H7-12+H2=C4H8-1+H     3.01E12     0.0   10600.0     !H_Abstraction
exact:      Cd_rad/NonDeC     H2
C4H7-11+CH4=C4H8-1+CH3  1.59E13     0.0   13700.0     !H_Abstraction
exact:      Cd_pri_rad     C_methane
C4H7-12+CH4=C4H8-1+CH3  1.59E13     0.0   13700.0     !H_Abstraction
estimate: (Average:)    Cd_rad/NonDeC     C_methane

!!! H-abstraction of CH2O
CH2O+C3H7-1=HCO+C3H8    5500.0      2.81  5860.0      !H_Abstraction
exact:      CO_pri     C_rad/H2/Cs
CH2O+CH2OH=HCO+CH3OH    3.140E+06   1.753 12532.12    !H_Abstraction
estimate: (Average:)    CO_pri     C_rad/H2/O
CH2O+CH3O=HCO+CH3OH     1.02E11     0.0   2980.0      !H_Abstraction
exact:      CO_pri     O_rad/NonDeC
CH2O+C4H9-1=HCO+nC4H10  5500.0      2.81  5860.0      !H_Abstraction
exact:      CO_pri     C_rad/H2/Cs
CH2O+C2H5=HCO+C2H6      5500.0      2.81  10860.0     !H_Abstraction
exact:      CO_pri     C_rad/H2/Cs
C3H6+HCO=aC3H5+CH2O     1.08E+07    1.9   19010.0
   ! Tsang, W.; "Chemical kinetic database for combustion chemistry.
Part 5.  Propene",
   !    J. Phys. Chem. Ref. Data (1991) v.20 221-273

!!! H-abstraction of C4H6-13
nC4H5+H2=C4H6-13+H            4.49E12     0.0   10300.0
      !H_Abstraction exact:   Cd_pri_rad     H2
iC4H5+H2=C4H6-13+H            2.37E12     0.0   18200.0
      !H_Abstraction exact:   Cd_rad/OneDe     H2
nC4H5+CH4=C4H6-13+CH3         1.59E14     0.0   13700.0
      !H_Abstraction exact:   Cd_pri_rad     C_methane
C4H6-13+CH3=iC4H5+CH4         5.156E13    0.0   16200.0
      !H_Abstraction exact:   Cd/H/OneDe     C_methyl

!!! H-abstraction of n-butanol
nC4H10O+C2H3=C4H9O-1+C2H4     0.21E13     0.0   10175.0
      !H_Abstraction estimate: (Average:)    C/H3/Cs     Cd_pri_rad
nC4H10O+C2H3=C4H9O-2+C2H4     1020.0      3.0   8820.0
      !H_Abstraction exact:     C/H2/NonDeC     Cd_pri_rad
nC4H10O+C2H3=C4H9O-3+C2H4     1020.0      3.0   8820.0
      !H_Abstraction exact:     C/H2/NonDeC     Cd_pri_rad
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nC4H10O+C2H3=C4H9O-4+C2H4     3020.0      3.1   8820.0
      !H_Abstraction estimate: (Average:)    C/H2/CsO     Cd_pri_rad
nC4H10O+C2H3=C4H9O-5+C2H4     14.4        3.1   6940.0
      !H_Abstraction exact:     O/H/NonDeC     Cd_pri_rad
nC4H10O+C2H=C4H9O-1+C2H2      1.806E12    0.0   0.0
      !H_Abstraction exact:     C/H3/Cs     Ct_rad
nC4H10O+C2H=C4H9O-2+C2H2      1.21E12     0.0   0.0
      !H_Abstraction exact:     C/H2/NonDeC     Ct_rad
nC4H10O+C2H=C4H9O-3+C2H2      1.21E12     0.0   0.0
      !H_Abstraction exact:     C/H2/NonDeC     Ct_rad
nC4H10O+C2H=C4H9O-4+C2H2      1.21E12     0.0   0.0
      !H_Abstraction estimate: (Average:)    C/H2/CsO     Ct_rad
nC4H10O+C2H=C4H9O-5+C2H2      1.21E12     0.0   0.0
      !H_Abstraction exact:     O/H/NonDeC     Ct_rad

nC4H8O+C2H5=C4H7OJ(8)+C2H6    3.800E11    0.0   7210.0
      !H_Abstraction estimate: (Average:) CO/H/NonDe     C_rad/H2/Cs
C2H4+C4H6-13=C6H10_CYC        6.825E10    0.0   23361.8
      !Diels_alder_addition estimate: (Average:)      ene_unsub_unsub
diene_unsub_unsub_out     diene_in_2H
!aC3H5+aC3H5=C6H10            3.150e+12   0.0   0.0
      !R_Recombination estimate:   C_rad/H2/Cd     C_rad/H2/Cd

! New value from KVG 10Sept2009
C4H6-13+C2H3=C6H9_1_2_5                    1.805900e+13      0.00E+00
      1.02E+04
C6H10+CH3=C6H9_1_2_5+CH4                   2.1200000e+13     0.00E+00
      1.16E+04
C6H10+C2H5=C6H9_1_2_5+C2H6                 1.2960000e+12     0.00E+00
      1.20E+04
C6H10+H=C6H9_1_2_5+H2                      2.3120000e+14     0.00E+00
      7.84E+03
C6H10+C2H3=C6H9_1_2_5+C2H4                 1.7560000e+13     0.00E+00
      6.72E+03
C6H10+aC3H5=C6H9_1_2_5+C3H6                9.9200000e+12     0.00E+00
      2.00E+04
C6H9_1_2_5=C6H9_CYC_1_3                    1.1400000e+11     0.00E+00
      2.22E+04
C6H10_CYC+CH3=C6H9_CYC_1_3+CH4             7.0000000e+13     0.00E+00
      1.45E+04
C6H10_CYC+C2H5=C6H9_CYC_1_3+C2H6           4.4000000e+12     0.00E+00
      1.56E+04
C6H10_CYC+H=C6H9_CYC_1_3+H2                1.0960000e+15     0.00E+00
      1.08E+04
C6H10_CYC+C2H3=C6H9_CYC_1_3+C2H4           5.8000000e+13     0.00E+00
      9.63E+03
C6H10_CYC+aC3H5=C6H9_CYC_1_3+C3H6          1.0800000e+13     0.00E+00
      2.04E+04
C6H8_CYC_1_4+CH3=C6H7_CYC_1_2+CH4          2.0800000e+13     0.00E+00
      9.79E+03
C6H8_CYC_1_4+C2H5=C6H7_CYC_1_2+C2H6        1.2280000e+12     0.00E+00
      9.25E+03
C6H8_CYC_1_4+H=C6H7_CYC_1_2+H2             3.2280000e+14     0.00E+00
      5.81E+03
C6H8_CYC_1_4+C2H3=C6H7_CYC_1_2+C2H4        1.7120000e+13     0.00E+00
      4.68E+03
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C6H8_CYC_1_4+aC3H5=C6H7_CYC_1_2+C3H6      8.4800000e+12     0.00E+00
      1.56E+04
C6H7_CYC_1_2+H=C6H8_CYC_1_4               5.0000000e+13     0.00E+00
      0.00E+00
benzene+H=C6H7_CYC_1_2                    2.3555460e+14     0.00E+00
      5.95E+03
C6H8_CYC_1_4+H=C6H9_CYC_1_3               1.5703640e+14     0.00E+00
      5.95E+03
benzene+CH3=C7H9                          1.4580000e+13     0.00E+00
      1.02E+04
benzene+C2H3=C8H9                         1.4580000e+13     0.00E+00
      1.02E+04
!C7H8+H=C7H9                              2.3555460e+14     0.00E+00
      5.95E+03
C8H8+H=C8H9                               2.3555460e+14     0.00E+00
      5.95E+03


C4H9O-4+C4H9O-4=nC4H10O+nC4H8O      2.3500000e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/CsO
O_Csrad

!MRH 22Jul2010: based on CH3CHO+HO2=H2O2+CH3CO
!nC4H8O+HO2=H2O2+C4H7OJ(8)    3.01E+12    0.0   11924.0     !Baulch et
al. J. Phys. Chem. Ref. Data 21 1992 411
nC4H8O+HO2=H2O2+C4H7OJ(8)     2.67E+09    0.95  5.64E+03    !Based on
estimate of C4H8O-enol2+HO2=H2O2+C4H7O-13

!C4H7OJ(8)+H2O2=nC4H8O+HO2          2.0954701e+05      2.07782
16457.00000        !H_Abstraction estimate: (Average:)  CO_rad/NonDe
O/H/NonDeO

nC4H8O+C4H9O-4=C4H7OJ(8)+nC4H10O    1.0533755e+08      1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/NonDe
C_rad/H/CsO
!HO2+C4H7OJ(8)=O2+nC4H8O                   3.0000000e+11      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Orad
CO_rad/NonDe
C4H9O-4+C4H7OJ(8)=nC4H8O+nC4H8O     1.8100000e+14      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
CO_rad/NonDe
C4H9O-4+C3H7-1=nC4H10O+C3H6         1.0260000e+14      -0.35000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/CsO
C/H2/Nd_Csrad
C4H7OJ(8)+C3H7-1=nC4H8O+C3H6        1.1401172e+13      -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  CO_rad/NonDe
C/H2/Nd_Csrad
!aC3H5+H2O2=C3H6+HO2                1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
C3H6+C4H9O-4=aC3H5+nC4H10O          1.9814540e+12      0.00000
16850.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H/CsO
aC3H5+nC4H8O=C3H6+C4H7OJ(8)         3.8000000e+11      0.00000
12210.00000        !H_Abstraction exact:   C_rad/H2/Cd     CO/H/NonDe
C4H9O-4+aC3H5=nC4H8O+C3H6           1.8100000e+13      0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
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C3H7-1+aC3H5=C3H6+C3H6              1.4500000e+12      0.00000     -
130.00000    !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cd
HO2+aC3H5=H2O2+aC3H4                6.0300000e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Csrad
C4H9O-4+aC3H5=nC4H10O+aC3H4         4.5800000e+12      -0.35000    -
130.00000    !Disproportionation estimate: (Average:)  C_rad/H/CsO
Cdpri_Csrad
C4H7OJ(8)+aC3H5=nC4H8O+aC3H4        5.4132535e+12      -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  CO_rad/NonDe
Cdpri_Csrad
aC3H5+aC3H5=C3H6+aC3H4              8.4300000e+10      0.00000     -
260.00000    !Disproportionation exact:   C_rad/H2/Cd     Cdpri_Csrad
nC4H8O+OH=C4H7OJ(8)+H2O                    1.0000000e+13      0.00000
0.00000      !H_Abstraction exact:   CO/H/NonDe     O_pri_rad
OH+aC3H5=H2O+aC3H4                  6.0300000e+12      0.00000
0.00000      !Disproportionation exact:   O_pri_rad     Cdpri_Csrad
C4H9O-4+C4H9O-2=nC4H8O+nC4H10O      2.3500000e+12      0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H/NonDeC
C4H9O-2+nC4H8O=nC4H10O+C4H7OJ(8)    1.0533755e+08      1.14500
6325.00000   !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
CO/H/NonDe
C3H7-1+C4H9O-2=C3H6+nC4H10O         5.1300000e+13      -0.35000
0.00000      !Disproportionation exact:   C/H2/Nd_Csrad
C_rad/H/NonDeC
C4H9O-2+C3H6=nC4H10O+aC3H5          2.8700000e+11      0.00000
12300.00000        !H_Abstraction exact:   C_rad/H/NonDeC     C/H3/Cd
aC3H5+C4H9O-2=aC3H4+nC4H10O         4.5800000e+12      -0.35000    -
130.00000    !Disproportionation exact:   Cdpri_Csrad     C_rad/H/NonDeC
HO2+nSPC(351)=H2O2+nSPC(385)        1.2100000e+13      0.00000
0.00000      !Disproportionation exact:   O_Csrad     O_rad/NonDeO
C4H9O-4+nSPC(351)=nC4H10O+nSPC(385)       2.3500000e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/CsO
O_Csrad
C4H7OJ(8)+nSPC(351)=nC4H8O+nSPC(385)      1.8100000e+14      0.00000
0.00000      !Disproportionation estimate: (Average:)  CO_rad/NonDe
O_Csrad
aC3H5+nSPC(351)=C3H6+nSPC(385)            1.8100000e+13      0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
OH+nSPC(351)=H2O+nSPC(385)          2.4100000e+13      0.00000
0.00000      !Disproportionation exact:   O_pri_rad     O_Csrad
C4H9O-2+nSPC(351)=nC4H10O+nSPC(385)       2.3500000e+12      0.00000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC     O_Csrad
O2+nSPC(351)=HO2+nSPC(385)    4.6826e+11 0.3321 -1.0635e+03 ! from Zador
et al calculation for CH3CHOH+O2=HO2+CH3CHO (consistent with RMG) edited
by MHS 04.27.11
!O2+nSPC(351)=HO2+nSPC(385)         2.2800000e+13      0.00000
0.00000      !Disproportionation_O2d exact:   O2d     O_Csrad
nC4H10O+CH2CHO=C4H9O-2+CH3CHO       4.3131427e+02      2.80500
11040.00000        !H_Abstraction estimate: (Average:)  C/H2/NonDeC
C_rad/H2/CO
nC4H10O+CH2CHO=C4H9O-4+CH3CHO       3.0397882e+06      1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/CsO
C_rad/H2/CO
nC4H8O+CH2CHO=C4H7OJ(8)+CH3CHO      3.8000000e+11      0.00000
7210.00000   !H_Abstraction estimate: (Average:)  CO/H/NonDe
C_rad/H2/CO
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CH2CHO+C4H9O-4=CH3CHO+nC4H8O        5.9463101e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H2/CO
O_Csrad
CH2CHO+C3H7-1=CH3CHO+C3H6           2.0088970e+12      0.00000     -
43.33333     !Disproportionation estimate: (Average:)  C_rad/H2/CO
C/H2/Nd_Csrad
CH2CHO+aC3H5=CH3CHO+aC3H4           2.8507052e+11      0.00000     -
195.00000    !Disproportionation estimate: (Average:)  C_rad/H2/CO
Cdpri_Csrad
CH2CHO+nSPC(351)=CH3CHO+nSPC(385)   5.9463101e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H2/CO
O_Csrad
HO2+CH2CHO=H2O2+CH2CO               7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Csrad
C4H9O-4+CH2CHO=nC4H10O+CH2CO        7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H/CsO
COpri_Csrad
C4H7OJ(8)+CH2CHO=nC4H8O+CH2CO             7.7460197e+12      -0.06091
-63.81982    !Disproportionation estimate: (Average:)  CO_rad/NonDe
COpri_Csrad
aC3H5+CH2CHO=C3H6+CH2CO             7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H2/Cd
COpri_Csrad
C4H9O-2+CH2CHO=nC4H10O+CH2CO        7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H/NonDeC
COpri_Csrad
CH2CHO+CH2CHO=CH3CHO+CH2CO          7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H2/CO
COpri_Csrad
aC3H5+O=aC3H4+OH                    7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  Cdpri_Csrad
O_atom_triplet
CH2CHO+O=CH2CO+OH                   7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
O_atom_triplet
nC4H8O+O=C4H7OJ(8)+OH               5.0000000e+12      0.00000
1790.00000   !H_Abstraction exact:   CO/H/NonDe     O_atom_triplet
C3H6+O=aC3H5+OH                     2.5650000e+04      3.05000
3123.00000   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_atom_triplet

C3H6O+CH3=CH4+C3H5OJ(8)       2.9200000e+04     2.29000e+00
      5.44000e+03 !H_Abstraction exact:   CO/H/NonDe     C_methyl
C3H6O+aC3H5=C3H6+C3H5OJ(8)    3.8000000e+11     0.00000
      7210.00000  !H_Abstraction exact:   C_rad/H2/Cd     CO/H/NonDe
C3H6O+OH=H2O+C3H5OJ(8)        1.0000000e+13     0.00000
      0.00000     !H_Abstraction exact:   CO/H/NonDe     O_pri_rad

!!! Benzene + Aromatics from S.Sharma HXD mechanism
!FULVENE
pC3H3+pC3H3=FULVENE  7.91665e+35 -6.8701 14720.4
C*C*CC*C*C=FULVENE  1.88495e+22 -3.31379 36126.
!C5H4CH3=FULVENE+H  4.45885e+37 -7.59833 39124.1
ME2CYBE=FULVENE  8.42691e+41 -8.45431 67599.9
C#CCCC#C=FULVENE  5.98668e+22 -3.2546 41961.7
```

```
!O2+C5H4CH3=HO2+FULVENE 7.5600000e+11   0.00000   0.00000
!Disproportionation_O2d exact:   O2d     Cmethyl_Csrad
C5H5CH2-1=FULVENE+H  1.07e+29   -5.32   32810.
C5H5CH2-2=FULVENE+H  1.35e+58   -13.11   73890.
FULVENE=benzene  1.75265e+18 -1.54824 75550.6
C5H5CH2-3=FULVENE+H  3.67e+43   -9.19   57330.
HCCO+C5H4CH3=HCCOH+FULVENE 7.2300000e+13   0.00000   0.00000
!Disproportionation estimate:   O_rad/OneDe     Cmethyl_Csrad
benzene+H=FULVENE+H  1.05e+43   -8.16   47790.

!benzene
pC3H3+pC3H3=benzene  4.97905e+23 -3.2692 16726.7

C5H5CH2-1=benzene+H  1.97796e+31 -6.06562 20629.6
C5H5CH2-2=benzene+H  9.25364e+43 -9.19115 55756.8
C6H5+H(+m)=benzene(+m) 1E14 0.0 0.0  !Wang&Frenklach 2000
   LOW/ 6.6E75  -16.3  7000./
   TROE/ 1.0 0.1 585 6113/
C7H8+H=benzene+CH3          1.20E+13 0.0 5148.0  ! Emdee 1992
!benzene+CH3=C6H5+CH4  2.0E12  0.0  15000. !Zhang 31
benzene+OH=C6H5+H2O            1.63E+08 1.42 1454.0 ! BaulCH 1992
benzene+OH=C6H5OH+H  1.3E13  0.0  10600. !Baulch 22
C6H5+H2=benzene+H 5.7e4  2.43  6280.0 !Mebel 1997

!C6H5
pC3H3+pC3H3=C6H5+H  377.683 3.10881 15554.7
C6H5+C2H2=C8H6+H 3.98E+13 0.0 10099.0  !Stein1989
!C6H5+C4H2=C8H6+C2H 2e13 0.0 0.0 !Frenklach 1984
!Replaced with C10H7 PES
!Kinetics from RMG, thermo from MRH/CFG
!PDepNetwork HCC-C(C6H5)=CH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C6H5              80.61 68.37 18.54 25.1  30.94 35.75 42.22 46.78
      52.97  !Burcat 07-Jan-2011
!     C4H2              113.13      59.15 17.18 19.78 21.53 22.84 24.83
      26.35 28.87
!     C8H6        75.92 79.88 30.22 38.09 44.4  49.42 56.62 61.72 69.02
!Burcat 07-Jan-2011
!     C2H               137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C8H6+C2H(+m)=C6H5+C4H2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C10H7)  deltaHrxn(T=298K) = -19.317280861892925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3109000e+01 -1.9370000e-01 -9.4573000e-02 /
CHEB / -6.4157000e-01 2.8516000e-01 1.3790000e-01 /
CHEB / -2.4741000e-01 -9.1641000e-02 -4.3948000e-02 /
CHEB / -2.8405000e-02 -1.9150000e-02 -5.2557000e-03 /
CHEB / 2.4252000e-02 2.5921000e-02 6.7084000e-03 /
```

```
C6H5+H=C6H4+H2    2.0E07  2.00   1000. !   Pau96 est
C6H5+OH=C6H5O+H 5.0E13 0.0 0.0 !Their estimate
C6H5+O2=C6H5O+O  2.6E13 0.0 6100. !frank 34
C6H5+OH=C6H4+H2O    1.0E07  2.00   1000. !   Pauwels 1995 est
C6H5(+m)=C6H4+H(+m) 4.3E12  0.62  77300.0 !Wang&Frenklach 2000
   LOW/ 1.0E84  -18.87  90100.0/
   TROE/ 0.902  696  358  3856/

!C6H4
C4H2+C2H2=C6H4 5E78  -19.31  67920.0 !Wang&Frenklach 2000

!C6H5O
C6H5O+H(+m)=C6H5OH(+m) 1.0E14  0.0  0.0 !Their estimate
   LOW /1.0E94  -21.84 13900./ !Wang 27
   TROE /0.043 304 60000 5896/
C6H5O=CO+C5H5 2.5E11 0.0 43800. !Baulch 30

!C5H5
C5H5+H=cyC5H6 1.0E14  0.0 0.0 !Their Estimate
cyC5H6+H=C5H5+H2 2.8E13 0.0 2000. !Roy 42
cyC5H6+CH3=C5H5+CH4 1.8E-1 4.0 0.0 !Zhong 39
cyC5H6+OH=C5H5+H2O 3.1E6 2.0 0.0 !Zhong 39
!C5H5+CH3=C5H4CH3+H 2.1425e-33   13.255   -16281.2
!MRH replaced with PLOG formatting;
! kinetics from S. Sharma and W.H. Green J.Phys.Chem.A 2009 113 (31)
8871-8882
! values in Table 8 & 9 were fit to modified Arrhenius format, for each
P, by MRH
! C5H4CH3 = R2 in Sharma paper
C5H5+CH3=C5H4CH3+H      1.0   0.0   0.0
PLOG / 0.01 1.2124e+16  -0.5779           10872.7     /
PLOG / 1    4.9108e+31  -4.8507           24772.8 /
PLOG / 10   1.2866e+47  -9.0246           39796.5 /
PLOG / 100  5.9632e+56  -11.5290    52599.6     /
pC3H3+C2H3=C5H5+H   9.63E+40 -7.8   28820.0   ! Marinov 1996
cyC5H6+aC3H5=C5H5+C3H6 6.0E12 0.0 0.0 !Their Esimate
C5H5+CH3=C5H5CH3_1 1.1596e55  -12.564  15802.3
C5H5+CH3=C5H5CH2-2+H 4.39e+35   -6.25   31240.
C5H5=pC3H3+C2H2  8.10807e+49 -10.3674 99054.3

!C6H5OH
C6H5+OH=C6H5OH  1.0E13  0.0 0.0 !Their Calculation
C6H5OH=cyC5H6+CO 1.0E12 0.0 61200. !Horn40

!C5H5CH3_1
C5H5CH3_1=C5H4CH3+H 9.78e+108   -27.45   126860.
C5H5CH3_1+H=C5H4CH3+H2 3.8192408e+07   1.85000   1265.00
!H_Abstraction estimate:   C/H/Cs     H_rad
C5H5CH3_1=C5H5CH3_2 1.62E+13  0.00  24110. !highp

!C5H5CH3_2
C5H5CH3_2+H=C5H5CH2-2+H2 1.2990000e+06   2.38000   2800.00
!H_Abstraction exact:   C/H3/Cd     H_rad
C5H5CH3_2+pC3H3=C5H5CH2-2+aC3H4 2.3190000e+13   0.00000   7500.00
!H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
C5H5CH3_2=C5H5CH3_3 25.10E+13 0.00  24480. !highp
```

```
!C6H5CH3 (C7H8)
C7H8+H=C6H5CH2+H2        3.98E+02 3.44 3120.0 ! Emdee 1992
C6H5CH2+H=C7H8           1.80E+14 0.0    0.0  ! Emdee 1992
C6H5+CH3=C7H8         4.0e12 0.0 0.0 !estimate
!C7H8+OH=C6H5CH2+H2O      1.26E+13 0.0 2583.0  ! Emdee 1992

!C6H5CH2
CH3CCCH2+pC3H3=C6H5CH2+H   3.00E+12 0.0     0.0 ! Marinov 1996
C4H5-113+pC3H3=C6H5CH2+H   3.00E+12 0.0     0.0 ! Marinov 1996

!C6H5C2H3 (C8H8)
c5h4chchch2=C8H8  3.966e+78      -19.527        98300.
C8H8+OH=C6H5CCH2+H2O 1.0e7 2.0 2000. ! Marinov 1996
C8H8+H=C6H5CCH2+H2  2.0e7 2.0 6000. ! Marinov 1996
!C6H5+C4H4=C8H8+C2H 3.2E11 0.0 1900. !Harris 1988
!Replaced with C10H9 PES
!Kinetics from RMG, thermo from MRH/CFG
!PDepNetwork HCC-CH(C6H5)-CH2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C6H5              80.61 68.37 18.54 25.1  30.94 35.75 42.22 46.78
      52.97  !Burcat 07-Jan-2011
!     C4H4              71.86 66.24 17.18 20.88 23.88 26.32 30.06 32.83
      37.25
!     C8H8        35.64 80.89 28.33 37.37 45.37 52.0  61.19 67.72 76.95
!Burcat 07-Jan-2011
!     C2H               137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C8H8+C2H(+m)=C6H5+C4H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C10H9)  deltaHrxn(T=298K) = -20.307463745992422 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2428000e+01 -6.8810000e-01 -1.6101000e-01 /
CHEB / 4.8111000e-01 8.4593000e-01 1.5134000e-01 /
CHEB / -8.9495000e-02 -3.9369000e-02 7.0976000e-02 /
CHEB / -6.3426000e-02 -1.1587000e-01 -4.4825000e-02 /
CHEB / -1.1770000e-02 -4.6614000e-02 -3.8131000e-02 /

C5H5+pC3H3=C8H8 3.111e+92       -22.68        70100.
C6H5+C2H3=C8H8 1.06e26 -4.0 5250. !Colket 1986
c5h4chchch2+H=C8H8+H 1.934e+51       -10.45        28650.

!C6H5CCH2
C6H5CCH2+OH=C8H6+H2O 2e13 0.0 0.0 ! Marinov 1996
C6H5CCH2+H=C8H6+H2  5.0e13 0.0 0.0 ! Marinov 1996

!C5H4CH3
C5H4CH3=benzene+H  8.58223e+50 -11.9776 62078.2
```

```
!C5H5CH2-1
C5H5CH2-1=C6H7_CYC_1_2  2.39827e+44 -10.6512 19219.5
C5H5CH2-1=C5H5CH2-3  9.22553e+27 -5.12362 28314.7
C5H5CH2-1=C5H5CH2-2  1.68659e+30 -5.9432 21537.5
C5H5+CH3=C5H5CH2-1+H  1.33e+28   -4.11   42920.

!C5H5CH2-2
C5H5CH2-2=C5H5CH2-3  1.08193e+41 -8.73397 44399.
C5H5CH2-2=C6H7_CYC_1_2  2.79922e+50 -11.8919 52747.6

!C5H5CH2-3
C5H5+CH3=C5H5CH2-3+H 6.09e+30   -4.91   31470.
C5H5CH2-3=benzene+H  1.37674e+46 -9.72349 57338.

!ME2CYBE
pC3H3+pC3H3=ME2CYBE  2.32156e+50 -11.4678 15943.4
C#CCCC#C=ME2CYBE  2.00342e+43 -9.4465 43814.8
C*C*CC*C*C=ME2CYBE  2.58846e+37 -7.95974 30649.4
ME2CYBE=benzene  2.13318e+18 -1.59114 70687.6

!c5h4chchch2
C5H5+pC3H3=c5h4chchch2 5.094e+113       -28.79        71540.

!cyC6H7 (C6H7_CYC_1_2)
C6H7_CYC_1_2=FULVENE+H  1.69e+48   -10.97   66100.
!C6H7_CYC_1_2=benzene+H  1.68849e+40 -8.4357 37790.3

!C6H9-1 (C6H9_1_2_5)
!C2H3+C4H6-13=C6H9-1 1.4902950e+02   3.00740   10170.80
!R_Addition_MultipleBond estimate:   Cd_pri_rad     Cd/H2_Cd/H/De
!C6H9-1=C5H6CH3  1.15416e+36 -7.71076 43627.7
!C6H9-1=cyC5H6+CH3 2.083e+29        -5.97        37680.
!C6H9-1=C6H9 4.0953959e+08   1.13807   34830.32   !intra_H_migration
estimate:   R4H_SDS     C_rad_out_2H     Cs_H_out_H/OneDe

!C#CCCC#C
pC3H3+pC3H3=C#CCCC#C  4.28058e+34 -6.86383 5241.53
C#CCCC#C=C*C*CC*C*C  1.58081e+25 -4.13369 32252.
C#CCCC#C=benzene  1.31782e+10 0.437128 48464.2

!C*C*CC*C*C
C*C*CC*C*C=benzene  1.357e-05 4.70794 38967.5
pC3H3+pC3H3=C*C*CC*C*C  2.12425e+35 -6.80657 9548.05

!CH3CCCH2
!iC4H5=CH3CCCH2 2.0476980e+08        1.13807     40830.32
!intra_H_migration estimate:   Others-R2H_S    C_rad_out_2H     XH_out
C4H6-12+H=CH3CCCH2+H2 2.9800000e+07   1.95000   8650.00   !H_AbstraCtiOn
exaCt:   Cd/H/NOnDeC     H_rad      fOrward rate: 1.8143804204191 58E12
reverse rate:  4.7165256606216717E8
!pC3H3+CH3CCCH2=aC3H4+C4H4-123 5.1149449e+13   -0.17306   -1.81
!DisprOpOrtiOnatiOn estimate:   Cd_pri_rad     CmetHyl_Cdrad
fOrward rate: 1.4610595205530184E13  reverse rate:  9.494046411698591E9
!pC3H3+CH3CCCH2=pC3H4+C4H4-123 5.1149449e+13   -0.17306   -1.81
!DisprOpOrtiOnatiOn estimate:   C_rad/H2/Ct     CmetHyl_Cdrad
fOrward rate: 1.4610595205530184E13  reverse rate:  5.238706651309827E9
```

```
pC3H3+CH3CCCH2=pC3H4+C4H4-123 2.349247757572718E13    -
0.19690476190476192     -1.5476190476190477     !Disproportionation
estimate: (Average:)    C_rad/H2/Ct     Cmethyl_Cdrad
      deltaHrxn(T=298K) = -32.346640453456104 kcal/mol
pC3H3+CH3CCCH2=aC3H4+C4H4-123 2.349247757572718E13    -
0.19690476190476192     -1.5476190476190477     !Disproportionation
estimate: (Average:)    Cd_pri_rad     Cmethyl_Cdrad
      deltaHrxn(T=298K) = -31.39666174663681 kcal/mol
CH3+CH3CCCH2=CH4+C4H4-123 5.1149449e+13   -0.17306   -1.81
!DisprOpOrtiOnatiOn estimate:   C_metHyl     CmetHyl_Cdrad      fOrward
rate: 1.4610595205530184E13  reverse rate:  2.908415160696778E7
!C4H4-123+H=CH3CCCH2 2.0000000e+13   0.00000     1200.00
!R_Addition_MultipleBond exact:   Cd/H2_Ca     H_rad

pC3H3+CH3=C3H2+CH4 6.4800000e+03   2.58000   14040.00   !H_AbstraCtiOn
exaCt:   Cd_pri     C_metHyl      fOrward rate: 5.453322912527577E9
reverse rate:  4.1727189736918315E7
CH4+HCCO=CH3+CH2CO      6.36e+14    0.0   13700.0     !RMG
C4H4+H=iC4H3+H2 2.9214e+13     0.0   9799.3 !cbsqb3

C4H4+OH=iC4H3+H2O 1.1100000e+06   2.00000   1450.00   !H_AbstraCtiOn
estimate:   Cd/H/OneDe     O_pri_rad      fOrward rate:
1.2918292687132297E12  reverse rate:  2.779866861708262E8
C4H4+OH=nC4H3+H2O 1.0260000e+13   0.00000   5940.00   !H_AbstraCtiOn
exaCt:   Cd_pri     O_pri_rad      fOrward rate: 1.2128158027992366E12
reverse rate:  1.640375724350831E10
!C4H5-113+H=C4H6-12     1.4157E13   -0.15 291.67      !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     H_rad
C4H6-1+CH3=C4H5-113+CH4 4.0000000e+11   0.00000   9500.00
!H_AbstraCtiOn estimate:   C/H2/OneDeC     C_metHyl      fOrward rate:
1.3149839414820711E10  reverse rate:  5.6084303938287236E7
C4H6-1+H=C4H5-113+H2 1.3980000e+05   2.36000   1110.00   !reduced by a
factor of 10
pC3H3+H=C3H2+H2       4.3782e+13 0.0     9493.9   ! CBSQB3

pC3H3+OH=C3H2+H2O     1.5025e+13 0.0        5107.7   ! CBSQB3
!C2H+C2H3=C4H4    1.0E14      0.0   0.0   !R_Recombination exact:
      Ct_rad     Cd_pri_rad
!iC4H3+H=C4H4     1.416E13    -0.15 291.67      !R_Recombination
estimate: (Average:)    Cd_rad/OneDe     H_rad
!nC4H3+H=C4H4     5.36E14     0.0   0.98  !R_Recombination exact:
      Cd_pri_rad     H_rad

!C3H7-1+C2H3=C5H10_1 6.9100000e+14  -7.50E-01   0.00E+00
C2H6+C5H9_1_4=C2H5+C5H10_1 4.0920000e+12  0.00E+00    1.80E+04
C3H6+C5H9_1_4=aC3H5+C5H10_1 9.0000000e+11       0.00E+00    1.35E+04
!H+C5H9_1_4=C5H10_1 5.4400000e+13   1.60E-01    0.00E+00
CH3+C5H10_1=CH4+C5H9_1_4 2.6070000e+13    0.00E+00    1.68E+04
H+C5H10_1=H2+C5H9_1_4 4.0800000e+14       0.00E+00    1.30E+04
C2H3+C5H10_1=C2H4+C5H9_1_4 2.1540000e+13  0.00E+00    1.19E+04
C5H9_1_4=C5H9_CYC 8.7100000e+10     0.00E+00    1.72E+04

C5H8_CYC_1+H=C5H9_CYC 7.8518200e+13       0.00E+00    5.95E+03

C5H8_CYC_1+CH3=C5H7_CYC_1_2+CH4 2.1200000e+13   0.00E+00    1.16E+04
C5H8_CYC_1+C2H5=C5H7_CYC_1_2+C2H6 1.2960000e+12       0.00E+00
      1.20E+04
```

```
C5H8_CYC_1+H=C5H7_CYC_1_2+H2 3.3120000e+14      0.00E+00    7.84E+03
C5H8_CYC_1+C2H3=C5H7_CYC_1_2+C2H4 1.7560000e+13       0.00E+00
      6.72E+03
C5H8_CYC_1+aC3H5=C5H7_CYC_1_2+C3H6 9.9200000e+12      0.00E+00
      2.00E+04
C5H8_CYC_1+C5H9_1_4=C5H7_CYC_1_2+C5H10_1 1.2960000e+12      0.00E+00
      1.20E+04
cyC5H6+H=C5H7_CYC_1_2 1.1091740e+14       0.00E+00    3.85E+03

!C4H9O-1=C4H9O-3    1.18E10    0.82    35100.    !intra_H_migration
exact:     Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeC
!C4H9O-1=C4H9O-2    1.938E10    0.89    35800.    !intra_H_migration
estimate: (Average:)    Others-R2H_S    C_rad_out_2H
Cs_H_out_H/(NonDeC/Cs)
!C4H9O-1=C4H9O-4    6.44E9    0.13    20700.    !intra_H_migration
estimate: (Average:)    R4H_SSS     C_rad_out_2H     Cs_H_out_H/NonDeO
!C4H9O-5=C4H9O-1    3.75E10    0.0    24400.    !intra_H_migration
exact:     R5H_SSSS     O_rad_out     Cs_H_out_2H
!C4H9O-5=C4H9O-2    2.00E11    0.0    26850.    !intra_H_migration
estimate: (Average:)    R4H_SSS     O_rad_out     Cs_H_out_H/NonDeC
!C4H9O-5=C4H9O-3    1.11E10    1.06    39526.7    !intra_H_migration
estimate: (Average:)    Others-R3H_SS    O_rad_out
Cs_H_out_H/(NonDeC/Cs)
!C4H9O-5=C4H9O-4    4.095E8    1.138    34789.75    !intra_H_migration
estimate: (Average:)    Others-R2H_S    O_rad_out
Cs_H_out_H/(NonDeC/Cs)

!C4H8O-enol+H=C4H7O_1_2+H2    1398000.0    2.36    1110.
!H_Abstraction exact:     C/H2/OneDeC     H_rad
C4H8O-enol2+H=C4H7O_1_2+H2    1398000.0    2.36    1110.
!H_Abstraction estimate: (Average:)    C/H2/OneDeO     H_rad
C4H8O-enol+CH3=C4H7O_1_2+CH4    5.46E13    0.0    10400.
!H_Abstraction exact:     C/H2/OneDeC     C_methyl
C4H8O-enol2+CH3=C4H7O_1_2+CH4    5.46E13    0.0    10400.
!H_Abstraction estimate: (Average:)    C/H2/OneDeO     C_methyl
C4H8O-enol+OH=C4H7O_1_2+H2O    3.173E9    0.95    5644.
!H_Abstraction estimate: (Average:)    C/H2/OneDeC     O_pri_rad
!C4H8O-enol2+OH=C4H7O_1_2+H2O    3.173E9    0.95    5644.
!H_Abstraction estimate: (Average:)    C/H2/OneDeO     O_pri_rad
C4H8O-enol2+OH=C4H7O_1_2+H2O  3.12E+06    2.0         298.757
      !Estimate based on C3H6+OH=H2O+aC3H5

!H-Abstractions rxns of nC4H8O by OH
!nC4H8O+OH=C4H7OJ(16)+H2O     3600000.0   2.0   860.  !H_Abstraction
exact:      C/H3/Cs     O_pri_rad
nC4H8O+OH=C4H7OJ(16)+H2O      1.88e+05    2.51  442.16      !Based on
C2H6+OH=H2O+C2H5 and C3H8+OH=H2O+nC3H7
nC4H8O+OH=C4H7OJ(13)+H2O      7900000.0   1.9   160.  !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad
!nC4H8O+OH=C4H7OJ(12)+H2O     3.173E9     0.95  5644. !H_Abstraction
estimate: (Average:)    C/H2/OneDeC     O_pri_rad

!2-BuOH rxns
CH3CH[OH]CHCH3+sBuOH=sBuOH+CH3C[OH]C2H5 1.7454741e+07        1.50500
14520.00000        !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
C/H/NDMustO
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sBuOH+CH3CH[O]C2H5=CH2CH[OH]C2H5+sBuOH 1.4220000e+12   0.00000
7000.00000   !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
CH3CH[O]C2H5+sBuOH=sBuOH+CH3C[OH]C2H5 2.5321927e+11    0.00000
9446.50000   !H_Abstraction estimate: (Average:)  O_rad/NonDeC
C/H/NDMustO
CH3CH[O]C2H5+sBuOH=sBuOH+CH3CH[OH]CHCH3 1.4500000e+11        0.00000
4570.00000   !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
sBuOH+CH3CH[O]C2H5=CH3CH[OH]CH2CH2+sBuOH 1.4220000e+12       0.00000
7000.00000   !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
CH2CH[OH]C2H5+sBuOH=sBuOH+CH3C[OH]C2H5 1.8806816e+10   0.83667
15186.66667        !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H/NDMustO
CH2CH[OH]C2H5+sBuOH=sBuOH+CH3CH[OH]CHCH3 3.0800000e+03       2.66000
10100.00000        !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
sBuOH+CH2CH[OH]C2H5=CH3CH[OH]CH2CH2+sBuOH 1.9770000e+03      2.71000
12920.00000        !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
CH3CH[OH]CH2CH2+sBuOH=sBuOH+CH3C[OH]C2H5 1.8806816e+10       0.83667
15186.66667        !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H/NDMustO
CH3CH[OH]CH2CH2+sBuOH=sBuOH+CH3CH[OH]CHCH3 3.0800000e+03     2.66000
10100.00000        !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
!CH3CH[OH]CHCH3=CH3C[OH]C2H5 7.7918556e+09       0.86750     39675.00000
       !intra_H_migration estimate: (Average:)  Others-R2H_S
C_rad_out_H/NonDeC     Cs_H_out_NDMustO
!CH3CH[O]C2H5=CH3CH[OH]CH2CH2 3.0000000e+11      0.00000     29400.00000
       !intra_H_migration exact:   R4H_SSS     O_rad_out     Cs_H_out_2H
!CH3CH[O]C2H5=CH2CH[OH]C2H5 1.4130000e+09        1.45000     42270.00000
       !intra_H_migration estimate: (Average:)  Others-R3H_SS
O_rad_out     Cs_H_out_2H
!CH3CH[O]C2H5=CH3CH[OH]CHCH3 1.1125324e+10       1.06333     39526.66667
       !intra_H_migration estimate: (Average:)  Others-R3H_SS
O_rad_out     Cs_H_out_H/NonDeC
!CH3CH[O]C2H5=CH3C[OH]C2H5 2.0476980e+08   1.13807     34789.75195
!intra_H_migration estimate: (Average:)  Others-R2H_S    O_rad_out
Others-Cs_H_out_Cs2
!CH2CH[OH]C2H5=CH3CH[OH]CH2CH2 7.6200000e+09     0.35000     19760.00000
       !intra_H_migration estimate: (Average:)  R4H_SSS     C_rad_out_2H
Cs_H_out_2H
!CH2CH[OH]C2H5=CH3CH[OH]CHCH3 1.1800000e+10      0.82000     35100.00000
       !intra_H_migration exact:   Others-R3H_SS    C_rad_out_2H
Cs_H_out_H/NonDeC
!CH2CH[OH]C2H5=CH3C[OH]C2H5 1.1074749e+10        0.85500     37575.00000
       !intra_H_migration estimate: (Average:)  Others-R2H_S
C_rad_out_2H     Cs_H_out_NDMustO
!CH3CH[OH]CH2CH2=CH3C[OH]C2H5 2.2564489e+10      0.71900     39020.00000
       !intra_H_migration estimate: (Average:)  Others-R3H_SS
C_rad_out_2H     Cs_H_out_NDMustO
!CH3CH[OH]CH2CH2=CH3CH[OH]CHCH3 1.9380000e+10    0.89000     35800.00000
       !intra_H_migration estimate: (Average:)  Others-R2H_S
C_rad_out_2H     Cs_H_out_H/(NonDeC/Cs)
!C2H4O+C2H5=CH2CH[OH]C2H5 2.4827386e+10    0.24400     10487.50000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/Nd_Cd/H2
C_rad/H2/Cs
!CH3+C2H4O=CH3CH[OH]CH2 1.3600000e+12      0.00000     10100.00000
!R_Addition_MultipleBond exact:   Cd/H/Nd_Cd/H2     C_methyl
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CH3C[OH]C2H5+C2H5O-2=sBuOH+C2H4O 8.5800000e+15   -1.10000    0.00000
!Disproportionation estimate: (Average:)  C_rad/NDMustO
Cmethyl_Csrad
CH3CH[OH]CHCH3+C2H5O-2=sBuOH+C2H4O 6.3300000e+14       -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
CH3CH[O]C2H5+C2H5O-2=sBuOH+C2H4O 7.2300000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeC     Cmethyl_Csrad
CH2CH[OH]C2H5+C2H5O-2=sBuOH+C2H4O 6.9000000e+13        -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
CH3CH[OH]CH2CH2+C2H5O-2=sBuOH+C2H4O 6.9000000e+13      -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
!C2H4O+CH3=HOCHC2H5 3.1000000e+12    0.00000     8500.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/H/Nd     C_methyl
!C3H6+OH=CH3CH[OH]CH2 2.7100000e+12        0.00000     0.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/Nd_Cd/H2
O_pri_rad



!C2H4O+H=C2H5O-2 1.0100000e+13       0.00000     2100.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/H/Nd     H_rad
!CH3CHO+C2H5=CH3CH[O]C2H5 7.9400000e+10    0.00000     6700.00000
!R_Addition_MultipleBond estimate: (Average:)  CO/H/Nd_O     C_rad/H2/Cs
CH3C[OH]C2H5+C2H5O-2=sBuOH+CH3CHO 3.4700000e+14        -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/NDMustO
O_Csrad
CH3CH[OH]CHCH3+C2H5O-2=sBuOH+CH3CHO 2.3500000e+12      0.00000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC     O_Csrad
CH3CH[O]C2H5+C2H5O-2=sBuOH+CH3CHO 2.4100000e+13        0.00000
0.00000      !Disproportionation exact:   O_rad/NonDeC     O_Csrad
CH2CH[OH]C2H5+C2H5O-2=sBuOH+CH3CHO 2.4100000e+12       0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
CH3CH[OH]CH2CH2+C2H5O-2=sBuOH+CH3CHO 2.4100000e+12     0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
sBuOH+OH=CH2CH[OH]C2H5+H2O 1.6000000e+06   1.60000     860.00000
!H_Abstraction exact:   O_pri_rad     C/H3/Cs
sBuOH+OH=CH3C[OH]C2H5+H2O 1.7000000e+06    1.60000     -1451.00000
!H_Abstraction estimate: (Average:)  C/H/NDMustO     O_pri_rad
sBuOH+OH=CH3CH[OH]CHCH3+H2O 1.9000000e+06        1.60000     160.00000
!H_Abstraction exact:   C/H2/NonDeC     O_pri_rad
sBuOH+OH=CH3CH[OH]CH2CH2+H2O 1.6000000e+06       1.50000     860.00000
!H_Abstraction exact:   O_pri_rad     C/H3/Cs
sBuOH+OH=CH3CH[O]C2H5+H2O 1.7300000e+01    3.00000     -1140.00000
!H_Abstraction exact:   O/H/NonDeC     O_pri_rad
OH+C2H5O-2=H2O+C2H4O 7.2300000e+13   0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     O_pri_rad
!H2CCCH3[OH]+CH3=CH3C[OH]C2H5 3.9900000e+12      0.00000    12000.00000
       !R_Addition_MultipleBond exact:   Cd/H2_Cd/Nd2     C_methyl
!H2CCCH3[OH]+H=CH3CH[OH]CH2 1.1700000e+13        0.00000     4700.00000
       !R_Addition_MultipleBond exact:   Cd/Nd2_Cd/H2     H_rad
CH3C[OH]C2H5+CH3CH[OH]CH2=sBuOH+H2CCCH3[OH] 1.0800000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/NDMustO
C/H/NdNd_Csrad
CH3CH[OH]CHCH3+CH3CH[OH]CH2=sBuOH+H2CCCH3[OH] 2.5600000e+13        -
0.35000      0.00000     !Disproportionation exact:   C_rad/H/NonDeC
C/H/NdNd_Csrad
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CH3CH[O]C2H5+CH3CH[OH]CH2=sBuOH+H2CCCH3[OH] 1.2100000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H/NdNd_Csrad
CH2CH[OH]C2H5+CH3CH[OH]CH2=sBuOH+H2CCCH3[OH] 8.4300000e+11   0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     C/H/NdNd_Csrad
CH3CH[OH]CH2CH2+CH3CH[OH]CH2=sBuOH+H2CCCH3[OH] 8.4300000e+11
0.00000      0.00000     !Disproportionation exact:   C_rad/H2/Cs
C/H/NdNd_Csrad
OH+CH3CH[OH]CH2=H2O+H2CCCH3[OH] 1.2100000e+13    0.00000     0.00000
!Disproportionation exact:   O_pri_rad     C/H/NdNd_Csrad

!sBuOH+H=CH2CH[OH]C2H5+H2 0.8840000e+08    1.75000     7510.00000
!H_Abstraction exact:   H_rad     C/H3/Cs
!sBuOH+H=CH3C[OH]C2H5+H2 1.8300000e+08     1.54000     5980.00000
!H_Abstraction estimate: (Average:)  C/H/NDMustO     H_rad
!sBuOH+H=CH3CH[OH]CHCH3+H2 1.6000000e+08   1.69000     4780.00000
!H_Abstraction exact:   C/H2/NonDeC     H_rad
!sBuOH+H=CH3CH[OH]CH2CH2+H2 0.8840000e+08        1.75000     7510.00000
       !H_Abstraction exact:   H_rad     C/H3/Cs
!sBuOH+H=CH3CH[O]C2H5+H2 8.7000000e+08     1.39000     10070.00000
!H_Abstraction exact:   O/H/NonDeC     H_rad

H+CH3CH[OH]CH2=H2+H2CCCH3[OH] 9.0400000e+11      0.00000     0.00000
!Disproportionation exact:   H_rad     C/H/NdNd_Csrad
H+C2H5O-2=H2+C2H4O 1.0830000e+13     0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     H_rad
H+C2H5O-2=H2+CH3CHO 6.0300000e+12    0.00000     0.00000
!Disproportionation exact:   H_rad     O_Csrad
!CH3+C3H6O-enol=CH3CH[OH]CHCH3 1.3600000e+12     0.00000     15100.00000
       !R_Addition_MultipleBond estimate: (Average:)  C_methyl
Cd/H/Nd_Cd/H/Nd
!C3H6O-enol+H=HOCHC2H5 1.0000000e+13       0.00000     2900.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/Nd_Cd/H/Nd     H_rad
CH3C[OH]C2H5+HOCHC2H5=sBuOH+C3H6O-enol 4.3200000e+14   -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/NDMustO
C/H2/Nd_Csrad
CH3CH[OH]CHCH3+HOCHC2H5=sBuOH+C3H6O-enol 1.0260000e+14       -0.35000
0.00000      !Disproportionation exact:   C/H2/Nd_Csrad
C_rad/H/NonDeC
CH3CH[O]C2H5+HOCHC2H5=sBuOH+C3H6O-enol 4.8200000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/Nd_Csrad
CH2CH[OH]C2H5+HOCHC2H5=sBuOH+C3H6O-enol 2.9000000e+12        0.00000
0.00000      !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cs
CH3CH[OH]CH2CH2+HOCHC2H5=sBuOH+C3H6O-enol 2.9000000e+12      0.00000
0.00000      !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cs
OH+HOCHC2H5=H2O+C3H6O-enol 4.8200000e+13   0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     O_pri_rad
H+HOCHC2H5=H2+C3H6O-enol 3.6200000e+12     0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     H_rad
!C4H8-1+OH=CH2CH[OH]C2H5 2.7100000e+12     0.00000     0.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/Nd_Cd/H2
O_pri_rad
!C2H5O-2+C2H4=CH3CH[OH]CH2CH2 3.4706748e+11      0.00000     10733.33333
       !R_Addition_MultipleBond estimate: (Average:)  C_rad/H/CsO
Cd/H2_Cd/H2
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CH3C[OH]C2H5+C2H5=sBuOH+C2H4 8.5800000e+15       -1.10000    0.00000
!Disproportionation estimate: (Average:)  C_rad/NDMustO
Cmethyl_Csrad
CH3CH[OH]CHCH3+C2H5=sBuOH+C2H4 6.3300000e+14     -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H/NonDeC
CH3CH[O]C2H5+C2H5=sBuOH+C2H4 7.2300000e+13       0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeC     Cmethyl_Csrad
CH2CH[OH]C2H5+C2H5=sBuOH+C2H4 6.9000000e+13      -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
CH3CH[OH]CH2CH2+C2H5=sBuOH+C2H4 6.9000000e+13    -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs

CH3+CH3CH[OH]CH2=CH4+H2CCCH3[OH] 6.0200000e+12   -0.32000    0.00000
!Disproportionation exact:   C_methyl     C/H/NdNd_Csrad
CH3+C2H5O-2=CH4+C2H4O 6.5700000e+14        -0.68000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_methyl
CH3+C2H5O-2=CH4+CH3CHO 2.4100000e+12       0.00000     0.00000
!Disproportionation exact:   C_methyl     O_Csrad
CH3+HOCHC2H5=CH4+C3H6O-enol 2.3000000e+13        -0.32000    0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_methyl
!C4H8-2+OH=CH3CH[OH]CHCH3 5.4200000e+12    0.00000     0.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/Nd_Cd/H/Nd
O_pri_rad

CH2CH[OH]C2H5+C2H6=sBuOH+C2H5 1.9540000e+04      2.71000     14920.00000
       !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
sBuOH+C2H5=CH3C[OH]C2H5+C2H6 1.8806816e+09       0.83667     11186.66667
       !H_Abstraction estimate: (Average:)  C/H/NDMustO     C_rad/H2/Cs
sBuOH+C2H5=CH3CH[OH]CHCH3+C2H6 3.0800000e+03     2.56000     12100.00000
       !H_Abstraction exact:   C_rad/H2/Cs     C/H2/NonDeC
CH3CH[OH]CH2CH2+C2H6=sBuOH+C2H5 1.9540000e+04    2.71000     14920.00000
       !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
CH3CH[O]C2H5+C2H6=sBuOH+C2H5 1.8440000e+13       0.00000     10000.00000
       !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC

C2H5+CH3CH[OH]CH2=C2H6+H2CCCH3[OH] 8.4300000e+11       0.00000
0.00000      !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cs
C2H5+C2H5O-2=C2H6+C2H4O 6.9000000e+13      -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
C2H5+C2H5O-2=C2H6+CH3CHO 2.4100000e+12     0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cs
C2H5+HOCHC2H5=C2H6+C3H6O-enol 2.9000000e+12      0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cs
CH3CHO+CH3=CH3CH-O-CH3 7.2990714e+11       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  OCO     C_methyl
C3H7-1+CH2CH[OH]C2H5=C3H6+sBuOH 2.9000000e+12    0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cs     C/H2/Nd_Csrad
C3H7-1+CH3C[OH]C2H5=C3H6+sBuOH 4.3200000e+14     -0.75000    0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/NDMustO
C3H7-1+CH3CH[OH]CHCH3=C3H6+sBuOH 1.0260000e+14   -0.35000    0.00000
!Disproportionation exact:   C_rad/H/NonDeC     C/H2/Nd_Csrad
C3H7-1+CH3CH[OH]CH2CH2=C3H6+sBuOH 2.9000000e+12        0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     C/H2/Nd_Csrad
C3H7-1+CH3CH[O]C2H5=C3H6+sBuOH 4.8200000e+13     0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     O_rad/NonDeC
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C4H8-1+CH3C[OH]C2H5=C4H7-24+sBuOH 3.0397882e+06        1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/NDMustO
C4H8-1+CH3CH[OH]CHCH3=C4H7-24+sBuOH 3.0397882e+06      1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/H/NonDeC
C4H8-1+CH3CH[O]C2H5=C4H7-24+sBuOH 3.1729268e+09        0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
O_rad/NonDeC
C4H8-1+CH2CH[OH]C2H5=C4H7-24+sBuOH 3.0397882e+06       1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/H2/Cs
C4H8-1+CH3CH[OH]CH2CH2=C4H7-24+sBuOH 3.0397882e+06     1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/H2/Cs
C4H8-1+C2H5=C4H7-24+C2H6 3.0397882e+06     1.88583     13448.33333
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     C_rad/H2/Cs
C4H8-1+OH=C4H7-24+H2O 3.1729268e+09        0.95000     5644.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     O_pri_rad
C2H5O-2+C4H7-24=C2H4O+C4H8-1 6.3300000e+14       -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
C3H7-1+C4H7-24=C3H6+C4H8-1 1.0260000e+14   -0.35000    0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H/OneDeC
C2H5O-2+C4H7-24=CH3CHO+C4H8-1 2.3500000e+12      0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/H/OneDeC
CH3CH[OH]CH2+C4H7-24=H2CCCH3[OH]+C4H8-1 2.5600000e+13        -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/H/OneDeC
HOCHC2H5+C4H7-24=C3H6O-enol+C4H8-1 1.0260000e+14       -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H/OneDeC
C2H5+C4H7-24=C2H4+C4H8-1 6.3300000e+14     -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
C4H8-2+CH3C[OH]C2H5=C4H7-24+sBuOH 2.9080000e+12        0.00000
10200.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/NDMustO
C4H8-2+CH3CH[OH]CHCH3=C4H7-24+sBuOH 5.7220000e+12      0.00000
10300.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
C4H8-2+CH3CH[O]C2H5=C4H7-24+sBuOH 6.8964034e+07        1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeC
C4H8-2+CH2CH[OH]C2H5=C4H7-24+sBuOH 6.3600000e+12       0.00000
10400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
C4H8-2+CH3CH[OH]CH2CH2=C4H7-24+sBuOH 3.3600000e+12     0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
!C4H8-2+CH3=C4H7-24+CH4 8.8240000e+02      2.92000     7160.00000
!H_Abstraction exact:   C/H3/Cd     C_methyl
C4H8-2+C2H5=C4H7-24+C2H6 1.3600000e+12     0.00000     12400.00000
!H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
C4H8-2+OH=C4H7-24+H2O 6.8964034e+07        1.75000     3789.37500
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_pri_rad
!C4H8-2+H=C4H7-24+H2 2.5980000e+06   2.38000     2800.00000
!H_Abstraction exact:   C/H3/Cd     H_rad
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C2H5O-2+C4H7-24=C2H4O+C4H8-2 6.8700000e+13       -0.35000    -130.00000
       !Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
C3H7-1+C4H7-24=C3H6+C4H8-2 2.9000000e+12   0.00000     -130.00000
!Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
C2H5O-2+C4H7-24=CH3CHO+C4H8-2 1.8100000e+13      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cd     O_Csrad
CH3CH[OH]CH2+C4H7-24=H2CCCH3[OH]+C4H8-2 7.8300000e+11        0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     C/H/NdNd_Csrad
HOCHC2H5+C4H7-24=C3H6O-enol+C4H8-2 2.9000000e+12       0.00000     -
130.00000    !Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
C2H5+C4H7-24=C2H4+C4H8-2 6.8700000e+13     -0.35000    -130.00000
!Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
C4H7-24+C4H8-1=C4H8-2+C4H7-24 3.0397882e+06      1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cd     C/H2/OneDeC
C4H7-14+sBuOH=C4H8-1+CH3C[OH]C2H5 1.8806816e+10        0.83667
15186.66667        !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H/NDMustO
C4H7-14+sBuOH=C4H8-1+CH3CH[OH]CHCH3 3.0800000e+03      2.66000
10100.00000        !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C4H8-1+CH3CH[O]C2H5=C4H7-14+sBuOH 1.4220000e+12        0.00000
7000.00000   !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
C4H8-1+CH2CH[OH]C2H5=C4H7-14+sBuOH 1.9770000e+03       2.71000
12920.00000        !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
C4H8-1+CH3CH[OH]CH2CH2=C4H7-14+sBuOH 1.9770000e+03     2.71000
12920.00000        !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
C4H7-14+C2H6=C4H8-1+C2H5 3.9540000e+03     2.71000     12920.00000
!H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
C2H5O-2+C4H7-14=C2H4O+C4H8-1 6.9000000e+13       -0.35000    0.00000
!Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
C3H7-1+C4H7-14=C3H6+C4H8-1 2.9000000e+12   0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cs     C/H2/Nd_Csrad
C2H5O-2+C4H7-14=CH3CHO+C4H8-1 2.4100000e+12      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cs     O_Csrad
CH3CH[OH]CH2+C4H7-14=H2CCCH3[OH]+C4H8-1 8.4300000e+11        0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     C/H/NdNd_Csrad
HOCHC2H5+C4H7-14=C3H6O-enol+C4H8-1 2.9000000e+12       0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     C/H2/Nd_Csrad
C2H5+C4H7-14=C2H4+C4H8-1 6.9000000e+13     -0.35000    0.00000
!Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
C4H7-14+C4H8-1=C4H8-1+C4H7-24 3.0397882e+06      1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cs     C/H2/OneDeC
C4H7-14+C4H8-2=C4H8-1+C4H7-24 3.3600000e+12      0.00000     12400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
C2H3+sBuOH=C2H4+CH3C[OH]C2H5 1.9500000e+13       0.00000     10200.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H/NDMustO
C2H3+sBuOH=C2H4+CH3CH[OH]CHCH3 1.0200000e+03     3.10000     8820.00000
       !H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
C2H3+sBuOH=C2H4+CH3CH[O]C2H5 1.4400000e+01       3.10000     6940.00000
       !H_Abstraction exact:   O/H/NonDeC     Cd_pri_rad
C2H3+sBuOH=C2H4+CH2CH[OH]C2H5 1.5107911e+13      0.00000     10175.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
C2H3+sBuOH=C2H4+CH3CH[OH]CH2CH2 1.5107911e+13    0.00000     10175.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
C2H5O-2+C2H3=C2H4O+C2H4 4.5600000e+14      -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C3H7-1+C2H3=C3H6+C2H4 2.4200000e+12        0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
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C2H5O-2+C2H3=CH3CHO+C2H4 3.0100000e+13     0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
CH3CH[OH]CH2+C2H3=H2CCCH3[OH]+C2H4 8.4300000e+11       0.00000
0.00000      !Disproportionation exact:   Cd_pri_rad     C/H/NdNd_Csrad
HOCHC2H5+C2H3=C3H6O-enol+C2H4 2.4200000e+12      0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
C2H5+C2H3=C2H4+C2H4 4.5600000e+14    -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C2H3+C4H8-1=C2H4+C4H7-24 1.0200000e+03     3.10000     8820.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H2/OneDeC
C2H3+C4H8-2=C2H4+C4H7-24 4.6380000e+13     0.00000     7500.00000
!H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
C2H3+C4H8-1=C2H4+C4H7-14 1.5107911e+13     0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
!C2H3+C2H4=C4H7-14 2.1800000e+13     0.00000     5200.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/H2     Cd_pri_rad
CH3C[OH]C2H5+C4H7-24=sBuOH+C4H6-13 8.5800000e+15       -1.10000
0.00000      !Disproportionation estimate: (Average:)  C_rad/NDMustO
Cmethyl_Csrad
CH3CH[OH]CHCH3+C4H7-24=sBuOH+C4H6-13 6.3300000e+14     -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
CH3CH[O]C2H5+C4H7-24=sBuOH+C4H6-13 7.2300000e+13       0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeC
Cmethyl_Csrad
CH2CH[OH]C2H5+C4H7-24=sBuOH+C4H6-13 6.9000000e+13      -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
CH3CH[OH]CH2CH2+C4H7-24=sBuOH+C4H6-13 6.9000000e+13    -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
CH3+C4H7-24=CH4+C4H6-13 6.5700000e+14      -0.68000    0.00000
!Disproportionation exact:   C_methyl     Cmethyl_Csrad
H+C4H7-24=H2+C4H6-13 1.0830000e+13   0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
C4H7-24+C4H7-24=C4H8-1+C4H6-13 6.3300000e+14     -0.70000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
C4H7-24+C4H7-24=C4H8-2+C4H6-13 6.8700000e+13     -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
!C4H6-13+H=C4H7-14 5.7000000e+13     0.00000     4300.00000
!R_Addition_MultipleBond exact:   Cd/H/De_Cd/H2     H_rad
CH3C[OH]C2H5+C4H7-14=sBuOH+C4H6-13 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/NDMustO
C/H2/De_Csrad
CH3CH[OH]CHCH3+C4H7-14=sBuOH+C4H6-13 1.1401172e+13     -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H/NonDeC
C/H2/De_Csrad
CH3CH[O]C2H5+C4H7-14=sBuOH+C4H6-13 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/De_Csrad
CH2CH[OH]C2H5+C4H7-14=sBuOH+C4H6-13 1.1401172e+13      -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/De_Csrad
CH3CH[OH]CH2CH2+C4H7-14=sBuOH+C4H6-13 1.1401172e+13    -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/De_Csrad
H+C4H7-14=H2+C4H6-13 1.1401172e+13   -0.07100    -2.16667
!Disproportionation estimate: (Average:)  H_rad     C/H2/De_Csrad
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C4H7-14+C4H7-24=C4H8-1+C4H6-13 6.9000000e+13     -0.35000    0.00000
!Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
C4H7-24+C4H7-14=C4H8-2+C4H6-13 1.1401172e+13     -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     C/H2/De_Csrad
C4H7-14+C4H7-14=C4H8-1+C4H6-13 1.1401172e+13     -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C_rad/H2/Cs     C/H2/De_Csrad
C2H3+C4H7-24=C2H4+C4H6-13 4.5600000e+14    -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C2H3+C4H7-14=C2H4+C4H6-13 1.1401172e+13    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  Cd_pri_rad     C/H2/De_Csrad
!CH3CH[OH]CH2=CH3C[OH]CH3 1.1074749e+10    0.85500     37575.00000
!intra_H_migration estimate: (Average:)  Others-R2H_S    C_rad_out_2H
Cs_H_out_NDMustO
!H2CCCH3[OH]+H=CH3C[OH]CH3 4.9400000e+13   0.00000     1500.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/Nd2     H_rad
CH3C[OH]CH3+CH2CH[OH]C2H5=H2CCCH3[OH]+sBuOH 1.3800000e+14    -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
CH3C[OH]CH3+CH3C[OH]C2H5=H2CCCH3[OH]+sBuOH 1.7160000e+16     -1.10000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/NDMustO
CH3C[OH]CH3+CH3CH[OH]CHCH3=H2CCCH3[OH]+sBuOH 1.2660000e+15   -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
CH3C[OH]CH3+CH3CH[OH]CH2CH2=H2CCCH3[OH]+sBuOH 1.3800000e+14        -
0.35000      0.00000     !Disproportionation exact:   C_rad/H2/Cs
Cmethyl_Csrad
CH3C[OH]CH3+CH3CH[O]C2H5=H2CCCH3[OH]+sBuOH 1.4460000e+14     0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/NonDeC
!CH3C[OH]CH3+OH=H2CCCH3[OH]+H2O 1.4460000e+14    0.00000     0.00000
!Disproportionation exact:   O_pri_rad     Cmethyl_Csrad
CH3C[OH]CH3+H=H2CCCH3[OH]+H2 2.1660000e+13       0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
CH3C[OH]CH3+C4H7-24=H2CCCH3[OH]+C4H8-1 1.2660000e+15   -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
CH3C[OH]CH3+C4H7-14=H2CCCH3[OH]+C4H8-1 1.3800000e+14   -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
CH3C[OH]CH3+C2H3=H2CCCH3[OH]+C2H4 9.1200000e+14        -0.70000
0.00000      !Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
CH3C[OH]CH3+CH3=H2CCCH3[OH]+CH4 1.3140000e+15    -0.68000    0.00000
!Disproportionation exact:   C_methyl     Cmethyl_Csrad
CH3C[OH]CH3+C4H7-24=H2CCCH3[OH]+C4H8-2 1.3740000e+14   -0.35000    -
130.00000    !Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
CH3C[OH]CH3+C2H5=H2CCCH3[OH]+C2H6 1.3800000e+14        -0.35000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
!acetone+H=CH3C[OH]CH3 7.2990714e+11       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  OCO     H_rad
CH3C[OH]C2H5+CH3C[OH]CH3=sBuOH+acetone 3.4700000e+14   -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/NDMustO
O_Csrad
CH3CH[OH]CHCH3+CH3C[OH]CH3=sBuOH+acetone 2.3500000e+12       0.00000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC     O_Csrad
CH3CH[O]C2H5+CH3C[OH]CH3=sBuOH+acetone 2.4100000e+13   0.00000
0.00000      !Disproportionation exact:   O_rad/NonDeC     O_Csrad
CH2CH[OH]C2H5+CH3C[OH]CH3=sBuOH+acetone 2.4100000e+12        0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
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CH3CH[OH]CH2CH2+CH3C[OH]CH3=sBuOH+acetone 2.4100000e+12      0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
CH3+CH3C[OH]CH3=CH4+acetone 2.4100000e+12        0.00000     0.00000
!Disproportionation exact:   C_methyl     O_Csrad
C2H5+CH3C[OH]CH3=C2H6+acetone 2.4100000e+12      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cs     O_Csrad
OH+CH3C[OH]CH3=H2O+acetone 2.4100000e+13   0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
H+CH3C[OH]CH3=H2+acetone 6.0300000e+12     0.00000     0.00000
!Disproportionation exact:   H_rad     O_Csrad
C4H7-24+CH3C[OH]CH3=C4H8-1+acetone 2.3500000e+12       0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
O_Csrad
C4H7-24+CH3C[OH]CH3=C4H8-2+acetone 1.8100000e+13       0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C4H7-14+CH3C[OH]CH3=C4H8-1+acetone 2.4100000e+12       0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
C2H3+CH3C[OH]CH3=C2H4+acetone 3.0100000e+13      0.00000     0.00000
!Disproportionation exact:   O_Csrad     Cd_pri_rad
pC3H5+sBuOH=C3H6+CH3C[OH]C2H5 8.9500000e+13      0.00000     6200.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H/NDMustO
pC3H5+sBuOH=C3H6+CH3CH[OH]CHCH3 1.0200000e+03    3.10000     8820.00000
       !H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
pC3H5+sBuOH=C3H6+CH3CH[O]C2H5 1.4400000e+01      3.10000     6940.00000
       !H_Abstraction exact:   O/H/NonDeC     Cd_pri_rad
pC3H5+sBuOH=C3H6+CH2CH[OH]C2H5 1.5107911e+13     0.00000     9175.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
pC3H5+sBuOH=C3H6+CH3CH[OH]CH2CH2 1.5107911e+13   0.00000     9175.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
pC3H5+C2H6=C3H6+C2H5 3.0215822e+13   0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
C2H5O-2+pC3H5=C2H4O+C3H6 4.5600000e+14     -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C3H7-1+pC3H5=C3H6+C3H6 2.4200000e+12       0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
C2H5O-2+pC3H5=CH3CHO+C3H6 3.0100000e+13    0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
CH3CH[OH]CH2+pC3H5=H2CCCH3[OH]+C3H6 8.4300000e+11      0.00000
0.00000      !Disproportionation exact:   Cd_pri_rad     C/H/NdNd_Csrad
CH3C[OH]CH3+pC3H5=H2CCCH3[OH]+C3H6 9.1200000e+14       -0.70000
0.00000      !Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
!pC3H5+OH=C3H6O-enol 1.4157154e+13   -0.15000    291.66667
!R_Recombination estimate: (Average:)  Cd_pri_rad     O_pri_rad
HOCHC2H5+pC3H5=C3H6O-enol+C3H6 2.4200000e+12     0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
C2H5+pC3H5=C2H4+C3H6 4.5600000e+14   -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
!CH3+pC3H5=C4H8-2 7.2300000e+13      0.00000     0.00000
!R_Recombination exact:   C_methyl     Cd_pri_rad
pC3H5+C4H8-1=C3H6+C4H7-24 1.0200000e+03    3.10000     8820.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H2/OneDeC
pC3H5+C4H8-2=C3H6+C4H7-24 4.6380000e+13    0.00000     7500.00000
!H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
pC3H5+C4H8-1=C3H6+C4H7-14 1.5107911e+13    0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
pC3H5+C2H4=C3H6+C2H3 5.8800000e+13   0.00000     13100.00000
!H_Abstraction exact:   Cd_pri     Cd_pri_rad
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C4H7-24+pC3H5=C4H6-13+C3H6 4.5600000e+14   -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C4H7-14+pC3H5=C4H6-13+C3H6 1.1401172e+13   -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     Cd_pri_rad
CH3C[OH]CH3+pC3H5=acetone+C3H6 3.0100000e+13     0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
CH3CHO+CH3C[OH]C2H5=CH3CO+sBuOH 1.0533755e+08    1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/NonDe     C_rad/NDMustO
CH3CHO+CH3CH[OH]CHCH3=CH3CO+sBuOH 1.0533755e+08        1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/NonDe
C_rad/H/NonDeC
CH3CHO+CH3CH[O]C2H5=CH3CO+sBuOH 3.0100000e+12    0.00000     11920.00000
       !H_Abstraction estimate: (Average:)  CO/H/NonDe     O_rad/NonDeC
CH3CHO+CH2CH[OH]C2H5=CH3CO+sBuOH 3.8000000e+11   0.00000     7210.00000
       !H_Abstraction estimate: (Average:)  CO/H/NonDe     C_rad/H2/Cs
CH3CHO+CH3CH[OH]CH2CH2=CH3CO+sBuOH 3.8000000e+11       0.00000
7210.00000   !H_Abstraction estimate: (Average:)  CO/H/NonDe
C_rad/H2/Cs
!CH3CO+H=CH3CHO 1.4157154e+13        -0.15000    291.66667
!R_Recombination estimate: (Average:)  CO_rad/NonDe     H_rad
C2H5O-2+CH3CO=C2H4O+CH3CHO 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_rad/NonDe
C3H7-1+CH3CO=C3H6+CH3CHO 1.1401172e+13     -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     CO_rad/NonDe
C2H5O-2+CH3CO=CH3CHO+CH3CHO 1.8100000e+14        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     CO_rad/NonDe
CH3CH[OH]CH2+CH3CO=H2CCCH3[OH]+CH3CHO 3.5218932e+12    -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
CO_rad/NonDe
CH3C[OH]CH3+CH3CO=H2CCCH3[OH]+CH3CHO 1.4130468e+14     -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/NonDe
HOCHC2H5+CH3CO=C3H6O-enol+CH3CHO 1.1401172e+13   -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     CO_rad/NonDe
C2H5+CH3CO=C2H4+CH3CHO 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_rad/NonDe
CH3CO+C4H8-1=CH3CHO+C4H7-24 7.5657121e+06        1.95000     16625.00000
       !H_Abstraction estimate: (Average:)  CO_rad/NonDe     C/H2/OneDeC
CH3CO+C4H8-2=CH3CHO+C4H7-24 2.9158025e+04        2.73500     17885.00000
       !H_Abstraction estimate: (Average:)  CO_rad/NonDe     C/H3/Cd
CH3CHO+C4H7-14=CH3CO+C4H8-1 3.8000000e+11        0.00000     7210.00000
       !H_Abstraction estimate: (Average:)  CO/H/NonDe     C_rad/H2/Cs
C4H7-24+CH3CO=C4H6-13+CH3CHO 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_rad/NonDe
C4H7-14+CH3CO=C4H6-13+CH3CHO 1.1401172e+13       -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     CO_rad/NonDe
!CH3+CH3CO=acetone 4.0400000e+15     -0.80000    0.00000
!R_Recombination exact:   C_methyl     CO_rad/NonDe
CH3C[OH]CH3+CH3CO=acetone+CH3CHO 1.8100000e+14   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     CO_rad/NonDe
CH3CHO+pC3H5=CH3CO+C3H6 8.1300000e+10      0.00000     3680.00000
!H_Abstraction exact:   Cd_pri_rad     CO/H/NonDe
!CH2CO+H=CH3CO 1.8833259e+13   0.00000     2900.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Ck     H_rad
CH3C[OH]C2H5+CH3CO=sBuOH+CH2CO 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/NDMustO
Cmethyl_COrad
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CH3CH[OH]CHCH3+CH3CO=sBuOH+CH2CO 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H/NonDeC
Cmethyl_COrad
CH3CH[O]C2H5+CH3CO=sBuOH+CH2CO 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_rad/NonDeC     Cmethyl_COrad
CH2CH[OH]C2H5+CH3CO=sBuOH+CH2CO 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cs     Cmethyl_COrad
CH3CH[OH]CH2CH2+CH3CO=sBuOH+CH2CO 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
Cmethyl_COrad
CH3+CH3CO=CH4+CH2CO 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_methyl     Cmethyl_COrad
C2H5+CH3CO=C2H6+CH2CO 7.0652342e+13        -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cs     Cmethyl_COrad
OH+CH3CO=H2O+CH2CO 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_pri_rad     Cmethyl_COrad
H+CH3CO=H2+CH2CO 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  H_rad     Cmethyl_COrad
C4H7-24+CH3CO=C4H8-1+CH2CO 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_COrad
C4H7-24+CH3CO=C4H8-2+CH2CO 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cmethyl_COrad
C4H7-14+CH3CO=C4H8-1+CH2CO 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cs     Cmethyl_COrad
C2H3+CH3CO=C2H4+CH2CO 7.0652342e+13        -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cd_pri_rad     Cmethyl_COrad
pC3H5+CH3CO=C3H6+CH2CO 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cd_pri_rad     Cmethyl_COrad
CH3CO+CH3CO=CH3CHO+CH2CO 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  CO_rad/NonDe     Cmethyl_COrad
C4H6-13+CH3=C2H5CHCHCH2 1.4600000e+13      0.00000     5700.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/H/De     C_methyl
H2CCCH3[OH]+CH3C[OH]C2H5=CH2C[OH]CH2+sBuOH 9.5400000e+12     0.00000
11200.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/NDMustO
H2CCCH3[OH]+CH3CH[OH]CHCH3=CH2C[OH]CH2+sBuOH 8.6100000e+11   0.00000
12300.00000        !H_Abstraction exact:   C_rad/H/NonDeC     C/H3/Cd
H2CCCH3[OH]+CH3CH[O]C2H5=CH2C[OH]CH2+sBuOH 3.4482017e+07     1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeC
H2CCCH3[OH]+CH2CH[OH]C2H5=CH2C[OH]CH2+sBuOH 1.6800000e+12    0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
H2CCCH3[OH]+CH3CH[OH]CH2CH2=CH2C[OH]CH2+sBuOH 1.6800000e+12
0.00000      12400.00000       !H_Abstraction exact:   C_rad/H2/Cs
C/H3/Cd
H2CCCH3[OH]+CH3=CH2C[OH]CH2+CH4 2.4120000e+02    2.92000     7160.00000
       !H_Abstraction exact:   C_methyl     C/H3/Cd
H2CCCH3[OH]+C2H5=CH2C[OH]CH2+C2H6 1.6800000e+12        0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
H2CCCH3[OH]+OH=CH2C[OH]CH2+H2O 3.4482017e+07     1.75000     3789.37500
       !H_Abstraction estimate: (Average:)  C/H3/Cd     O_pri_rad
H2CCCH3[OH]+H=CH2C[OH]CH2+H2 1.2990000e+05       2.38000     2800.00000
       !H_Abstraction exact:   H_rad     C/H3/Cd
!CH2C[OH]CH2+H=H2CCCH3[OH] 5.0000000e+13   0.00000     0.00000
!R_Recombination estimate: (Average:)  C_rad/H2/Cd     H_rad
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C2H5O-2+CH2C[OH]CH2=C2H4O+H2CCCH3[OH] 6.8700000e+13    -0.35000    -
130.00000    !Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
C3H7-1+CH2C[OH]CH2=C3H6+H2CCCH3[OH] 2.9000000e+12      0.00000     -
130.00000    !Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
C2H5O-2+CH2C[OH]CH2=CH3CHO+H2CCCH3[OH] 1.8100000e+13   0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
CH3CH[OH]CH2+CH2C[OH]CH2=H2CCCH3[OH]+H2CCCH3[OH] 7.8300000e+11
0.00000      -130.00000        !Disproportionation exact:   C_rad/H2/Cd
C/H/NdNd_Csrad
CH3C[OH]CH3+CH2C[OH]CH2=H2CCCH3[OH]+H2CCCH3[OH] 1.3740000e+14      -
0.35000      -130.00000        !Disproportionation exact:   C_rad/H2/Cd
Cmethyl_Csrad
HOCHC2H5+CH2C[OH]CH2=C3H6O-enol+H2CCCH3[OH] 2.9000000e+12    0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
C2H5+CH2C[OH]CH2=C2H4+H2CCCH3[OH] 6.8700000e+13        -0.35000    -
130.00000    !Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
CH2C[OH]CH2+C4H8-1=H2CCCH3[OH]+C4H7-24 3.0397882e+06   1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
C/H2/OneDeC
CH2C[OH]CH2+C4H8-2=H2CCCH3[OH]+C4H7-24 3.4680000e+13   0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
H2CCCH3[OH]+C4H7-14=CH2C[OH]CH2+C4H8-1 1.6800000e+12   0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
H2CCCH3[OH]+C2H3=CH2C[OH]CH2+C2H4 2.3190000e+13        0.00000
7500.00000   !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
C4H7-24+CH2C[OH]CH2=C4H6-13+H2CCCH3[OH] 6.8700000e+13        -0.35000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
C4H7-14+CH2C[OH]CH2=C4H6-13+H2CCCH3[OH] 1.1401172e+13        -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C/H2/De_Csrad
C_rad/H2/Cd
CH3C[OH]CH3+CH2C[OH]CH2=acetone+H2CCCH3[OH] 1.8100000e+13    0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
H2CCCH3[OH]+pC3H5=CH2C[OH]CH2+C3H6 2.3190000e+13       0.00000
7500.00000   !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
H2CCCH3[OH]+CH3CO=CH2C[OH]CH2+CH3CHO 1.4579012e+04     2.73500
17885.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
CO_rad/NonDe
CH3CO+CH2C[OH]CH2=CH2CO+H2CCCH3[OH] 7.0652342e+13      -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
C_rad/H2/Cd
H2CCCH3[OH]+CH3C[OH]C2H5=CH2C[O]CH3+sBuOH 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/NDMustO
H2CCCH3[OH]+CH3CH[OH]CHCH3=CH2C[O]CH3+sBuOH 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/NonDeC
H2CCCH3[OH]+CH3CH[O]C2H5=CH2C[O]CH3+sBuOH 1.7300000e+01      3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeC
H2CCCH3[OH]+CH2CH[OH]C2H5=CH2C[O]CH3+sBuOH 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
H2CCCH3[OH]+CH3CH[OH]CH2CH2=CH2C[O]CH3+sBuOH 1.4867217e+03   2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
H2CCCH3[OH]+CH3=CH2C[O]CH3+CH4 1.0700000e+04     2.04000     18850.00000
       !H_Abstraction exact:   O/H/OneDe     C_methyl
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H2CCCH3[OH]+C2H5=CH2C[O]CH3+C2H6 1.4867217e+03   2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cs
H2CCCH3[OH]+OH=CH2C[O]CH3+H2O 1.7300000e+01      3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     O_pri_rad
H2CCCH3[OH]+H=CH2C[O]CH3+H2 1.3000000e+11        0.82000     7750.00000
       !H_Abstraction exact:   O/H/OneDe     H_rad
!CH2C[O]CH3+H=H2CCCH3[OH] 1.4157154e+13    -0.15000    291.66667
!R_Recombination estimate: (Average:)  O_rad/OneDe     H_rad
C2H5O-2+CH2C[O]CH3=C2H4O+H2CCCH3[OH] 7.2300000e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C3H7-1+CH2C[O]CH3=C3H6+H2CCCH3[OH] 4.8200000e+13       0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_rad/OneDe
C2H5O-2+CH2C[O]CH3=CH3CHO+H2CCCH3[OH] 1.7076592e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
O_rad/OneDe
CH3CH[OH]CH2+CH2C[O]CH3=H2CCCH3[OH]+H2CCCH3[OH] 1.2100000e+13
0.00000      0.00000     !Disproportionation estimate: (Average:)
C/H/NdNd_Csrad     O_rad/OneDe
!CH3C[OH]CH3+CH2C[O]CH3=H2CCCH3[OH]+H2CCCH3[OH] 1.4460000e+14
0.00000      0.00000     !Disproportionation estimate: (Average:)
Cmethyl_Csrad     O_rad/OneDe
HOCHC2H5+CH2C[O]CH3=C3H6O-enol+H2CCCH3[OH] 4.8200000e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_rad/OneDe
C2H5+CH2C[O]CH3=C2H4+H2CCCH3[OH] 7.2300000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     O_rad/OneDe
CH2C[O]CH3+C4H8-1=H2CCCH3[OH]+C4H7-24 1.1729268e+09    0.95000
10644.00000        !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H2/OneDeC
CH2C[O]CH3+C4H8-2=H2CCCH3[OH]+C4H7-24 1.8964034e+06    1.75000
10789.37500        !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H3/Cd
H2CCCH3[OH]+C4H7-14=CH2C[O]CH3+C4H8-1 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
H2CCCH3[OH]+C2H3=CH2C[O]CH3+C2H4 1.4400000e+01   3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_pri_rad
C4H7-24+CH2C[O]CH3=C4H6-13+H2CCCH3[OH] 7.2300000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C4H7-14+CH2C[O]CH3=C4H6-13+H2CCCH3[OH] 1.1401172e+13   -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/De_Csrad
O_rad/OneDe
CH2C[O]CH3+sBuOH=acetone+CH3C[OH]C2H5 1.8806816e+10    0.83667
15186.66667        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H/NDMustO
CH2C[O]CH3+sBuOH=acetone+CH3CH[OH]CHCH3 4.3131427e+02        2.80500
11040.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H2/NonDeC
acetone+CH3CH[O]C2H5=CH2C[O]CH3+sBuOH 6.8964034e+07    1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/CO
O_rad/NonDeC
CH2C[O]CH3+sBuOH=acetone+CH2CH[OH]C2H5 1.9770000e+03   2.71000
12920.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cs
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CH2C[O]CH3+sBuOH=acetone+CH3CH[OH]CH2CH2 1.9770000e+03       2.71000
12920.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cs
acetone+CH3=CH2C[O]CH3+CH4 1.8814906e+06   1.75273     17532.12121
!H_Abstraction estimate: (Average:)  C/H3/CO     C_methyl
CH2C[O]CH3+C2H6=acetone+C2H5 3.9540000e+03       2.71000     12920.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     C/H3/Cs
acetone+OH=CH2C[O]CH3+H2O 3.1020000e+06    2.20000     7000.00000
!H_Abstraction exact:   C/H3/CO     O_pri_rad
acetone+H=CH2C[O]CH3+H2 4.5514336e+05      2.31000     7947.50000
!H_Abstraction estimate: (Average:)  C/H3/CO     H_rad
CH2C[O]CH3+C4H8-1=acetone+C4H7-24 3.0397882e+06        1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H2/OneDeC
CH2C[O]CH3+C4H8-2=acetone+C4H7-24 1.7434638e+13        0.00000
17333.33333        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cd
CH2C[O]CH3+C4H8-1=acetone+C4H7-14 1.9770000e+03        2.71000
12920.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cs
acetone+C2H3=CH2C[O]CH3+C2H4 3.0215822e+13       0.00000     18175.00000
       !H_Abstraction estimate: (Average:)  C/H3/CO     Cd_pri_rad
!CH2C[O]CH3+H=acetone 5.0000000e+13        0.00000     0.00000
!R_Recombination estimate: (Average:)  C_rad/H2/CO     H_rad
C2H5O-2+CH2C[O]CH3=C2H4O+acetone 3.4509736e+13   -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/CO
C3H7-1+CH2C[O]CH3=C3H6+acetone 2.0088970e+12     0.00000     -43.33333
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     C_rad/H2/CO
C2H5O-2+CH2C[O]CH3=CH3CHO+acetone 5.9463101e+12        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H2/CO
CH3C[OH]CH3+CH2C[O]CH3=acetone+H2CCCH3[OH] 1.7076592e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
O_rad/OneDe
CH3CH[OH]CH2+CH2C[O]CH3=H2CCCH3[OH]+acetone 5.4183717e+11    0.00000
-43.33333    !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/H2/CO
HOCHC2H5+CH2C[O]CH3=C3H6O-enol+acetone 2.0088970e+12   0.00000     -
43.33333     !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H2/CO
C2H5+CH2C[O]CH3=C2H4+acetone 3.4509736e+13       -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/CO
C4H7-24+CH2C[O]CH3=C4H6-13+acetone 3.4509736e+13       -0.23333    -
43.33333     !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H2/CO
C4H7-14+CH2C[O]CH3=C4H6-13+acetone 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/De_Csrad
C_rad/H2/CO
CH3C[OH]CH3+CH2C[O]CH3=acetone+acetone 5.9463101e+12   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H2/CO
H2CCCH3[OH]+pC3H5=CH2C[O]CH3+C3H6 1.4400000e+01        3.10000
6940.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
Cd_pri_rad
acetone+pC3H5=CH2C[O]CH3+C3H6 3.0215822e+13      0.00000     9175.00000
       !H_Abstraction estimate: (Average:)  C/H3/CO     Cd_pri_rad
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H2CCCH3[OH]+CH3CO=CH2C[O]CH3+CH3CHO 2.0954701e+05      2.07782
16457.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
CO_rad/NonDe
CH2C[O]CH3+CH3CHO=acetone+CH3CO 3.8000000e+11    0.00000     7210.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     CO/H/NonDe
!CH2CO+CH3=CH2C[O]CH3  2.8149495e+12       0.00000     7856.66667
!R_Addition_MultipleBond estimate: (Average:)  Ck_Cd/H2     C_methyl
!DUPLICATE
!CH2CO+CH3=CH2C[O]CH3  1.9263655e+11       0.04067     9290.00000
!R_Addition_MultipleBond estimate: (Average:)  Ck_O     C_methyl
!DUPLICATE
CH3CO+CH2C[O]CH3=CH2CO+H2CCCH3[OH] 7.0652342e+13       -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
O_rad/OneDe
CH3CO+CH2C[O]CH3=CH2CO+acetone 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     C_rad/H2/CO
H2CCCH3[OH]+CH2C[OH]CH2=CH2C[O]CH3+H2CCCH3[OH] 1.4867217e+03
2.38600      9690.00000        !H_Abstraction estimate: (Average:)
O/H/OneDe     C_rad/H2/Cd
CH2C[O]CH3+H2CCCH3[OH]=acetone+CH2C[OH]CH2 8.7173191e+12     0.00000
17333.33333        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cd
!CH2C[O]CH3=CH2C[OH]CH2 1.4130000e+09      1.45000     42270.00000
!intra_H_migration estimate: (Average:)  R3H_SS_2Cd     O_rad_out
Cs_H_out_2H
CH2C[O]CH3+H2CCCH3[OH]=acetone+CH2C[O]CH3 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
O/H/OneDe
C2H4O+CH3C[OH]C2H5=CH2CHO+sBuOH 1.4867217e+03    2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/NDMustO
C2H4O+CH3CH[OH]CHCH3=CH2CHO+sBuOH 1.4867217e+03        2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/NonDeC
C2H4O+CH3CH[O]C2H5=CH2CHO+sBuOH 1.7300000e+01    3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     O_rad/NonDeC
C2H4O+CH2CH[OH]C2H5=CH2CHO+sBuOH 1.4867217e+03   2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cs
C2H4O+CH3CH[OH]CH2CH2=CH2CHO+sBuOH 1.4867217e+03       2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
C2H4O+CH3=CH2CHO+CH4 9.0700000e+04   2.04000     10850.00000
!H_Abstraction exact:   O/H/OneDe     C_methyl
C2H4O+C2H5=CH2CHO+C2H6 1.4867217e+03       2.38600     9690.00000
!H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cs
C2H5O-2+CH2CHO=C2H4O+C2H4O 7.2300000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     O_rad/OneDe
C2H4O+OH=CH2CHO+H2O 1.7300000e+01    3.40000     -1140.00000
!H_Abstraction estimate: (Average:)  O/H/OneDe     O_pri_rad
C2H4O+H=CH2CHO+H2 1.3000000e+11      0.82000     7750.00000
!H_Abstraction exact:   O/H/OneDe     H_rad
CH2CHO+sBuOH=CH3CHO+CH3C[OH]C2H5 1.8806816e+10   0.83667     15186.66667
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     C/H/NDMustO
CH2CHO+sBuOH=CH3CHO+CH3CH[OH]CHCH3 4.3131427e+02       2.80500
11040.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H2/NonDeC
CH3CHO+CH3CH[O]C2H5=CH2CHO+sBuOH 3.4482017e+07   1.75000     3789.37500
       !H_Abstraction estimate: (Average:)  C/H3/CO     O_rad/NonDeC
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CH3CHO+CH2CH[OH]C2H5=CH2CHO+sBuOH 9.4074532e+06        1.75273
12532.12121        !H_Abstraction estimate: (Average:)  C/H3/CO
C_rad/H2/Cs
CH3CHO+CH3CH[OH]CH2CH2=CH2CHO+sBuOH 9.4074532e+06      1.75273
12532.12121        !H_Abstraction estimate: (Average:)  C/H3/CO
C_rad/H2/Cs
CH3CHO+C2H5=CH2CHO+C2H6 9.4074532e+06      1.75273     12532.12121
!H_Abstraction estimate: (Average:)  C/H3/CO     C_rad/H2/Cs
C2H5O-2+CH2CHO=CH3CHO+C2H4O 1.7076592e+13        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     O_rad/OneDe
C2H5O-2+CH2CHO=CH3CHO+CH3CHO 5.9463101e+12       0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/H2/CO
CH3CH[OH]CH2+CH2CHO=H2CCCH3[OH]+C2H4O 1.2100000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/OneDe
CH3C[OH]CH3+CH2CHO=H2CCCH3[OH]+C2H4O 1.4460000e+14     0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
CH3CH[OH]CH2+CH2CHO=H2CCCH3[OH]+CH3CHO 5.4183717e+11   0.00000     -
43.33333     !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/H2/CO
CH3C[OH]CH3+CH2CHO=H2CCCH3[OH]+CH3CHO 6.9019473e+13    -0.23333    -
43.33333     !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H2/CO
HOCHC2H5+CH2CHO=C3H6O-enol+C2H4O 4.8200000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     O_rad/OneDe
HOCHC2H5+CH2CHO=C3H6O-enol+CH3CHO 2.0088970e+12        0.00000     -
43.33333     !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H2/CO
C2H5+CH2CHO=C2H4+CH3CHO 3.4509736e+13      -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/CO
CH2CHO+C4H8-1=C2H4O+C4H7-24 3.1729268e+09        0.95000     15644.00000
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     C/H2/OneDeC
CH2CHO+C4H8-1=CH3CHO+C4H7-24 3.0397882e+06       1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     C/H2/OneDeC
C2H4O+C4H7-24=CH2CHO+C4H8-2 1.4867217e+03        2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cd
CH2CHO+C4H8-2=CH3CHO+C4H7-24 1.7434638e+13       0.00000     17333.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     C/H3/Cd
C2H4O+C4H7-14=CH2CHO+C4H8-1 1.4867217e+03        2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cs
CH3CHO+C4H7-14=CH2CHO+C4H8-1 9.4074532e+06       1.75273     12532.12121
       !H_Abstraction estimate: (Average:)  C/H3/CO     C_rad/H2/Cs
C2H4O+C2H3=CH2CHO+C2H4 1.4400000e+01       3.10000     6940.00000
!H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_pri_rad
CH3CHO+C2H3=CH2CHO+C2H4 1.5107911e+13      0.00000     9175.00000
!H_Abstraction estimate: (Average:)  C/H3/CO     Cd_pri_rad
C4H7-14+CH2CHO=C4H6-13+C2H4O 1.1401172e+13       -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     O_rad/OneDe
C4H7-24+CH2CHO=C4H6-13+CH3CHO 3.4509736e+13      -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/CO
C4H7-14+CH2CHO=C4H6-13+CH3CHO 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     C_rad/H2/CO
CH3C[OH]CH3+CH2CHO=acetone+C2H4O 1.7076592e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     O_rad/OneDe
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CH3C[OH]CH3+CH2CHO=acetone+CH3CHO 5.9463101e+12        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H2/CO
C2H4O+pC3H5=CH2CHO+C3H6 1.4400000e+01      3.10000     6940.00000
!H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_pri_rad
CH3CHO+pC3H5=CH2CHO+C3H6 1.5107911e+13     0.00000     9175.00000
!H_Abstraction estimate: (Average:)  C/H3/CO     Cd_pri_rad
C2H4O+CH3CO=CH2CHO+CH3CHO 2.0954701e+05    2.07782     16457.00000
!H_Abstraction estimate: (Average:)  O/H/OneDe     CO_rad/NonDe
CH2CHO+CH3CHO=CH3CHO+CH3CO 3.8000000e+11   0.00000     7210.00000
!H_Abstraction estimate: (Average:)  C_rad/H2/CO     CO/H/NonDe
!CH2CHO=CH3CO 2.0476980e+08    1.13807     34789.75195
!intra_H_migration estimate: (Average:)  Others-R2H_S    C_rad_out_2H
CO_H_out
CH2CHO+CH2CH[OH]C2H5=CH2CO+sBuOH 7.7460197e+12   -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H2/Cs
CH2CHO+CH3C[OH]C2H5=CH2CO+sBuOH 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/NDMustO
CH2CHO+CH3CH[OH]CHCH3=CH2CO+sBuOH 7.7460197e+12        -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H/NonDeC
CH2CHO+CH3CH[OH]CH2CH2=CH2CO+sBuOH 7.7460197e+12       -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H2/Cs
CH2CHO+CH3CH[O]C2H5=CH2CO+sBuOH 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     O_rad/NonDeC
CH3CO+CH2CHO=CH2CO+C2H4O 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     O_rad/OneDe
CH2CHO+CH2CHO=CH2CO+C2H4O 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     O_rad/OneDe
CH2CHO+pC3H5=CH2CO+C3H6 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     Cd_pri_rad
CH3CO+CH2CHO=CH2CO+CH3CHO 2.3550781e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     C_rad/H2/CO
CH2CHO+CH2C[OH]CH2=CH2CO+H2CCCH3[OH] 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H2/Cd
CH2CHO+CH2C[O]CH3=CH2CO+H2CCCH3[OH] 7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
O_rad/OneDe
CH2CHO+C4H7-24=CH2CO+C4H8-1 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H/OneDeC
CH2CHO+C4H7-14=CH2CO+C4H8-1 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H2/Cs
CH2CHO+C2H3=CH2CO+C2H4 7.7460197e+12       -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     Cd_pri_rad
CH2CHO+CH3=CH2CO+CH4 7.7460197e+12   -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_methyl
CH2CHO+C4H7-24=CH2CO+C4H8-2 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H2/Cd
CH2CHO+C2H5=CH2CO+C2H6 7.7460197e+12       -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H2/Cs
CH2CHO+CH2C[O]CH3=CH2CO+acetone 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     C_rad/H2/CO
C2H4O+CH2C[OH]CH2=CH2CHO+H2CCCH3[OH] 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cd
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CH2CHO+H2CCCH3[OH]=CH3CHO+CH2C[OH]CH2 8.7173191e+12    0.00000
17333.33333        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cd
C2H4O+CH2C[O]CH3=CH2CHO+H2CCCH3[OH] 1.7300000e+01      3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/OneDe
CH2CHO+H2CCCH3[OH]=CH3CHO+CH2C[O]CH3 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
O/H/OneDe
C2H4O+CH2C[O]CH3=CH2CHO+acetone 1.4867217e+03    2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/CO
CH3CHO+CH2C[O]CH3=CH2CHO+acetone 9.4074532e+06   1.75273     12532.12121
       !H_Abstraction estimate: (Average:)  C/H3/CO     C_rad/H2/CO
CH2CHO+C2H4O=CH3CHO+CH2CHO 1.4867217e+03   2.38600     9690.00000
!H_Abstraction estimate: (Average:)  C_rad/H2/CO     O/H/OneDe
acetone+CH3=CH3-O-C(CH3)2 7.2990714e+11    0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  OCO     C_methyl
HCCO+C2H6=CH2CO+C2H5 3.0215822e+13   0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
HCCO+C4H8-1=CH2CO+C4H7-24 1.0200000e+03    3.10000     8820.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H2/OneDeC
HCCO+C4H8-2=CH2CO+C4H7-24 1.6380000e+13    0.00000     9500.00000
!H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
HCCO+C4H8-1=CH2CO+C4H7-14 1.5107911e+13    0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
CH2CO+C2H3=HCCO+C2H4 2.9400000e+13   0.00000     13100.00000
!H_Abstraction exact:   Cd_pri_rad     Cd_pri
CH2CO+pC3H5=HCCO+C3H6 2.9400000e+13        0.00000     13100.00000
!H_Abstraction exact:   Cd_pri_rad     Cd_pri
HCCO+CH3CHO=CH2CO+CH3CO 2.1300000e+10      0.00000     3680.00000
!H_Abstraction exact:   CO/H/NonDe     Cd_pri_rad
HCCO+H=CH2CO 5.3600000e+14     0.00000     980.00000   !R_Recombination
exact:   H_rad     Cd_pri_rad
C2H5O-2+HCCO=C2H4O+CH2CO 4.5600000e+14     -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C3H7-1+HCCO=C3H6+CH2CO 2.4200000e+12       0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
C2H5O-2+HCCO=CH3CHO+CH2CO 3.0100000e+13    0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
CH3CH[OH]CH2+HCCO=H2CCCH3[OH]+CH2CO 8.4300000e+11      0.00000
0.00000      !Disproportionation exact:   Cd_pri_rad     C/H/NdNd_Csrad
CH3C[OH]CH3+HCCO=H2CCCH3[OH]+CH2CO 9.1200000e+14       -0.70000
0.00000      !Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
HOCHC2H5+HCCO=C3H6O-enol+CH2CO 2.4200000e+12     0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     C/H2/Nd_Csrad
C2H5+HCCO=C2H4+CH2CO 4.5600000e+14   -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C4H7-24+HCCO=C4H6-13+CH2CO 4.5600000e+14   -0.70000    0.00000
!Disproportionation exact:   Cd_pri_rad     Cmethyl_Csrad
C4H7-14+HCCO=C4H6-13+CH2CO 1.1401172e+13   -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     Cd_pri_rad
CH3C[OH]CH3+HCCO=acetone+CH2CO 3.0100000e+13     0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
CH3CO+HCCO=CH2CO+CH2CO 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     Cd_pri_rad
CH2CHO+HCCO=CH2CO+CH2CO 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     Cd_pri_rad
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HCCO+H2CCCH3[OH]=CH2CO+CH2C[OH]CH2 2.3190000e+13       0.00000
17500.00000        !H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
HCCO+H2CCCH3[OH]=CH2CO+CH2C[O]CH3 1.4400000e+01        3.10000
6940.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad
O/H/OneDe
!HCCO+acetone=CH2CO+CH2C[O]CH3 3.0215822e+13     0.00000     9175.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/CO
HCCO+acetone=CH2CO+CH2C[O]CH3 5.08e-01    4.09  6.66e+03    !CBS-QB3
HCCO+C2H4O=CH2CO+CH2CHO 1.4400000e+01      3.10000     6940.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     O/H/OneDe
HCCO+CH3CHO=CH2CO+CH2CHO 1.5107911e+13     0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/CO

!sBuOH=C4H8-2+H2O   4.50e+08   1.35   66.61e+03 !CBS-QB3 w/1dHR (cis)
!    DUP
!sBuOH=C4H8-2+H2O   7.08e+08   1.29   65.66e+03 !CBS-QB3 w/1dHR (trans)
!    DUP

!sBuOH+CH3=CH2CH[OH]C2H5+CH4 1.3400000e+06       1.80000     11050.00000
       !H_Abstraction exact:   C_methyl     C/H3/Cs
!sBuOH+CH3=CH3C[OH]C2H5+CH4 6.7400000e+05        1.83000     8940.00000
       !H_Abstraction estimate: (Average:)  C/H/NDMustO     C_methyl
!sBuOH+CH3=CH3CH[OH]CHCH3+CH4 1.0000000e+06      1.77000     8530.00000
       !H_Abstraction exact:   C/H2/NonDeC     C_methyl
!sBuOH+CH3=CH3CH[OH]CH2CH2+CH4 4.3400000e+05     1.70000     11050.00000
       !H_Abstraction exact:   C_methyl     C/H3/Cs
!sBuOH+CH3=CH3CH[O]C2H5+CH4 .3903E+05 2.0 7525.57      !H_Abstraction
exact:   C_methane     O_rad/NonDeC

O2+CH3C[OH]C2H5=HO2+MEK 4.6826e+11 0.3321 -1.0635e+03 !from rate
calculated by Zador et al for CH3CHOH+O2=HO2+CH3CHO (consistent with
RMG) edited by MHS 04.27.11
!O2+CH3C[OH]C2H5=HO2+MEK 2.2800000e+13     0.00000     0.00000
!Disproportionation_O2d exact:   O2d     O_Csrad
OH+CH3C[OH]C2H5=H2O+MEK 2.4100000e+13      0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
CH3C[OH]C2H5+CH3CH[OH]CHCH3=MEK+sBuOH 2.3500000e+12    0.00000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC     O_Csrad
CH3+CH3C[OH]C2H5=CH4+MEK 2.4100000e+12     0.00000     0.00000
!Disproportionation exact:   C_methyl     O_Csrad
CH3CH[O]C2H5+C2H3=MEK+C2H4 8.4300000e+11   0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H/NdNd_Orad     Cd_pri_rad
CH3C[OH]C2H5+C2H3=MEK+C2H4 3.0100000e+13   0.00000     0.00000
!Disproportionation exact:   Cd_pri_rad     O_Csrad
H+CH3C[OH]C2H5=H2+MEK 6.0300000e+12        0.00000     0.00000
!Disproportionation exact:   H_rad     O_Csrad
H+CH3CH[O]C2H5=H2+MEK 9.0400000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  H_rad     C/H/NdNd_Orad
CH3C[O]cHCH3+H2O2=MEK+HO2 2.9734435e+03    2.38600     9690.00000
!H_Abstraction estimate: (Average:)  C_rad/H/OneDeC     O/H/NonDeO
CH3C[O]cHCH3+sBuOH=MEK+CH3C[OH]C2H5 1.7454741e+07      1.50500
14520.00000        !H_Abstraction estimate: (Average:)  C_rad/H/OneDeC
C/H/NDMustO
MEK+OH=CH3C[O]cHCH3+H2O 3.1729268e+09      0.95000     5644.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     O_pri_rad
HO2+CH3C[O]cHCH3=O2+MEK 3.0000000e+11      0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     C_rad/H/OneDeC
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C2H5O-2+CH3C[O]cHCH3=CH3CHO+MEK 2.3500000e+12    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/H/OneDeC
C2H5+CH3C[O]cHCH3=C2H4+MEK 6.3300000e+14   -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
CH3CH[O]C2H5+CH3C[O]cHCH3=MEK+MEK 9.7450092e+12        -0.35500    -
10.83333     !Disproportionation estimate: (Average:)  C/H/NdNd_Orad
C_rad/H/OneDeC
CH3C[OH]C2H5+CH3C[O]cHCH3=MEK+MEK 2.3500000e+12        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/OneDeC
CH3C[O]cHCH3+sBuOH=MEK+CH3CH[OH]CHCH3 3.0400000e+01    3.19000
10310.00000        !H_Abstraction estimate: (Average:)  C_rad/H/OneDeC
C/H2/NonDeC
MEK+CH3CH[OH]CH2CH2=CH3C[O]cHCH3+sBuOH 3.0397882e+06   1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/H2/Cs
MEK+CH3CH[O]C2H5=CH3C[O]cHCH3+sBuOH 3.1729268e+09      0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
O_rad/NonDeC
CH3C[O]cHCH3+C4H8-2=MEK+C4H7-24 9.1200000e+12    0.00000     21400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H/OneDeC
CH3C[O]cHCH3+C4H8-1=MEK+C4H7-24 3.0397882e+06    1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H/OneDeC
C/H2/OneDeC
C4H7-24+CH3C[O]cHCH3=C4H6-13+MEK 6.3300000e+14   -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
CH3C[O]cHCH3+CH3CHO=MEK+CH3CO 1.0533755e+08      1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  C_rad/H/OneDeC
CO/H/NonDe
CH3CO+CH3C[O]cHCH3=CH2CO+MEK 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad
C_rad/H/OneDeC
MEK+C2H3=CH3C[O]cHCH3+C2H4 1.0200000e+03   3.10000     8820.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     Cd_pri_rad
MEK+H=CH3C[O]cHCH3+H2 1.3980000e+06        2.36000     10110.00000
!H_Abstraction exact:   C/H2/OneDeC     H_rad

CH2CH[OH]C2H5+C3H6=sBuOH+aC3H5      5.6E11      0.0   12400.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
CH3C[OH]C2H5+C3H6=sBuOH+aC3H5       3.18E12     0.0   11200.
      !H_Abstraction estimate: (Average:) C_rad/NDMustO     C/H3/Cd
CH3CH[OH]CHCH3+C3H6=sBuOH+aC3H5     2.87E11     0.0   12300.
      !H_Abstraction exact:   C_rad/H/NonDeC     C/H3/Cd
CH3CH[OH]CH2CH2+C3H6=sBuOH+aC3H5    5.6E11      0.0   12400.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
CH3CH[O]C2H5+C3H6=sBuOH+aC3H5       1.15E7      1.75  3789.4
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/Cd

CH2CH[OH]C2H5+C2H5OH=sBuOH+C2H5O-2        1.52e6      1.886 9448.34
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H2/CsO
sBuOH+C2H5O-2=CH3C[OH]C2H5+C2H5OH         1.745E7     1.505 14520.
      !H_Abstraction estimate: (Average:) C/H/NDMustO     C_rad/H/CsO
CH3CH[OH]CHCH3+C2H5OH=sBuOH+C2H5O-2       1.52e6      1.886 9448.34
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/CsO
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CH3CH[OH]CH2CH2+C2H5OH=sBuOH+C2H5O-2      1.52e6      1.886 9448.34
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H2/CsO
CH3CH[O]C2H5+C2H5OH=sBuOH+C2H5O-2         1.586E9     0.95  5644.
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/CsO

!MEK+H=CH3C[OH]C2H5     1.0E12      0.18  6585.1
      !R_Addition_MultipleBond estimate: (Average:)   OCO     H_rad
!CH3+C3H6O=CH3CH[O]C2H5 3.16E10     0.0   11510.
      !R_Addition_MultipleBond estimate: (Average:)   C_methyl
CO/H/Nd_O
!MEK+H=CH3CH[O]C2H5     1.00E11     0.0   11900.
      !R_Addition_MultipleBond estimate: (Average:)   CO/Nd2_O     H_rad

!MEK rxns: H-Abstractions
cH2C[O]C2H5+H2=MEK+H          1.563E12    0.0   21133.3
      !H_Abstraction estimate: (Average:) C_rad/H2/CO     H2

CH3C[O]CH2cH2+H2=MEK+H        4.57E11     0.0   14800.
      !H_Abstraction exact:   C_rad/H2/Cs     H2
MEK+OH=cH2C[O]C2H5+H2O        1.551E6     2.2   10000.
      !H_Abstraction exact:   C/H3/CO     O_pri_rad

MEK+OH=CH3C[O]CH2cH2+H2O      3.600E6     2.0   860.
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
MEK+CH3=cH2C[O]C2H5+CH4       1.407E6     1.75  12532.12
      !H_Abstraction estimate: (Average:) C/H3/CO     C_methyl
MEK+CH3=CH3C[O]cHCH3+CH4      1.46E13     0.0   18400.
      !H_Abstraction exact:   C/H2/OneDeC     C_methyl
MEK+CH3=CH3C[O]CH2cH2+CH4     8.340E5     1.9   11050.
      !H_Abstraction exact:   C/H3/Cs     C_methyl
MEK+C2H3=cH2C[O]C2H5+C2H4     1.511E13    0.0   9175.
      !H_Abstraction estimate: (Average:) C/H3/CO     Cd_pri_rad

MEK+C2H3=CH3C[O]CH2cH2+C2H4   1.511E13    0.0   9175.
      !H_Abstraction estimate: (Average:) C/H3/Cs     Cd_pri_rad
cH2C[O]C2H5+C2H6=MEK+C2H5     659.0       2.71  12920.
      !H_Abstraction estimate: (Average:) C_rad/H2/CO     C/H3/Cs
MEK+C2H5=CH3C[O]cHCH3+C2H6    3.040E6     1.886 15448.3
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     C_rad/H2/Cs
CH3C[O]CH2cH2+C2H6=MEK+C2H5   659.0       2.71  12920.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
cH2C[O]C2H5+C3H6=MEK+aC3H5    2.906E12    0.0   17333.3
      !H_Abstraction estimate: (Average:) C_rad/H2/CO     C/H3/Cd
CH3C[O]cHCH3+C3H6=MEK+aC3H5   1.52E12     0.0   21400.
      !H_Abstraction exact:   C_rad/H/OneDeC     C/H3/Cd
CH3C[O]CH2cH2+C3H6=MEK+aC3H5  5.6E11      0.0   12400.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
!MEK rxns: R-Recombinations
!CH3+C3H5OJ(8)=MEK                  4.04E15     -0.8  0.0
      !R_Recombination exact:       C_methyl     CO_rad/NonDe
!cH2C[O]C2H5+H=MEK                  5.00E13     0.0   0.0
      !R_Recombination estimate: (Average:)     C_rad/H2/CO     H_rad
!CH2C[O]CH3+CH3=MEK           2.487E15    -0.9  250.
      !R_Recombination estimate: (Average:)     C_rad/H2/CO     C_methyl
!CH3C[O]CH2cH2+H=MEK          1.0E14      0.0   0.0
      !R_Recombination exact:       C_rad/H2/Cs     H_rad
!MEK rxns: Disproportionations
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HO2+cH2C[O]C2H5=O2+MEK        3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/CO

HO2+CH3C[O]CH2cH2=O2+MEK      3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
!MEK rxns: Insertions
!C3H8+CO=MEK                          538.0       3.29  104500.
      !1,2_Insertion estimate: (Average:) C_methyl_C_pri     CO_birad

!MEKenol2 rxns: H-Abstractions
cHC[OH]C2H5+H2=MEKenol2+H                 4.49E12     0.0   10300.
      !H_Abstraction exact:   Cd_pri_rad     H2
MEKenol2+H=CH2C[OH]cHCH3+H2           1.398E6     2.36  1110.
      !H_Abstraction exact:   C/H2/OneDeC     H_rad
CH2C[OH]CH2cH2+H2=MEKenol2+H          4.57E11     0.0   14800.
      !H_Abstraction exact:   C_rad/H2/Cs     H2
MEKenol2+H=cH2C[O]C2H5+H2                 1.3E11      0.82  7750.
      !H_Abstraction exact:   O/H/OneDe     H_rad
MEKenol2+OH=cHC[OH]C2H5+H2O           1.026E13    0.0   5940.
      !H_Abstraction exact:   Cd_pri     O_pri_rad
MEKenol2+OH=CH2C[OH]cHCH3+H2O         3.173E9     0.95  5644.
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_pri_rad
MEKenol2+OH=CH2C[OH]CH2cH2+H2O            3.600E6     2.0   860.
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
MEKenol2+OH=cH2C[O]C2H5+H2O           17.3        3.4   -1140.
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_pri_rad
cHC[OH]C2H5+CH4=MEKenol2+CH3          1.59E14     0.0   13700.
      !H_Abstraction exact:   Cd_pri_rad     C_methane
MEKenol2+CH3=CH2C[OH]cHCH3+CH4            5.46E13     0.0   10400.
      !H_Abstraction exact:   C/H2/OneDeC     C_methyl
MEKenol2+CH3=CH2C[OH]CH2cH2+CH4           834000.0    1.9   11050.
      !H_Abstraction exact:   C/H3/Cs     C_methyl
MEKenol2+CH3=cH2C[O]C2H5+CH4          90700.0     2.04  10850.
      !H_Abstraction exact:   O/H/OneDe     C_methyl
cHC[OH]C2H5+C2H4=MEKenol2+C2H3            1.47E13     0.0   13100.
      !H_Abstraction exact:   Cd_pri_rad     Cd_pri
MEKenol2+C2H3=CH2C[OH]cHCH3+C2H4          1020        3.1   8820.
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     Cd_pri_rad
MEKenol2+C2H3=CH2C[OH]CH2cH2+C2H4   1.51E13     0.0   9175.
      !H_Abstraction estimate: (Average:) C/H3/Cs     Cd_pri_rad
MEKenol2+C2H3=cH2C[O]C2H5+C2H4            14.4        3.1   6940.
      !H_Abstraction estimate: (Average:) O/H/OneDe     Cd_pri_rad
cHC[OH]C2H5+C2H6=MEKenol2+C2H5            5.036E12    0.0   9175.
      !H_Abstraction estimate: (Average:) Cd_pri_rad     C/H3/Cs
MEKenol2+C2H5=CH2C[OH]cHCH3+C2H6          3.040E6     1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     C_rad/H2/Cs
CH2C[OH]CH2cH2+C2H6=MEKenol2+C2H5   659.0       2.71  12920.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
MEKenol2+C2H5=cH2C[O]C2H5+C2H6            1486.7      2.386 9690.
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/Cs
cHC[OH]C2H5+C3H6=MEKenol2+aC3H5           7.73E12     0.0   7500.
      !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
MEKenol2+aC3H5=CH2C[OH]cHCH3+C3H6   3.040E6     1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     C_rad/H2/Cd
CH2C[OH]CH2cH2+C3H6=MEKenol2+aC3H5  5.6E11      0.0   12400.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
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MEKenol2+aC3H5=cH2C[O]C2H5+C3H6           1486.7      2.386 9690.
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/Cd
!MEKenol2 rxns: Beta-scissions
!MEKenol2+H=CH3C[OH]C2H5      4.94E13     0.0   1500.
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/Nd2     H_rad
!MEKenol2+H=CH2CH[OH]C2H5     1.17E13     0.0   4700.
      !R_Addition_MultipleBond exact:     Cd/Nd2_Cd/H2     H_rad
!MEKenol2 rxns: R-Recombinations
!cHC[OH]C2H5+H=MEKenol2 5.36E14     0.0   980.  !R_Recombination exact:
      Cd_pri_rad     H_rad
!C2H3O-2+C2H5=MEKenol2  1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     C_rad/H2/Cs
!C4H7-12+OH=MEKenol2          1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     O_pri_rad
!CH2C[OH]CH2+CH3=MEKenol2     2.487E15    -0.9  250.  !R_Recombination
estimate: (Average:)    C_rad/H2/Cd     C_methyl
!CH2C[OH]cHCH3+H=MEKenol2     5.00E13     0.0   0.0   !R_Recombination
estimate: (Average:)    C_rad/H/OneDeC     H_rad
!CH2C[OH]CH2cH2+H=MEKenol2    1.0E14      0.0   0.0   !R_Recombination
exact:      C_rad/H2/Cs     H_rad
!cH2C[O]C2H5+H=MEKenol2 1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    O_rad/OneDe     H_rad
!MEKenol2 rxns: Disproportionations
HO2+cHC[OH]C2H5=O2+MEKenol2   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     Cd_pri_rad
HO2+CH2C[OH]cHCH3=O2+MEKenol2 3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/OneDeC
HO2+CH2C[OH]CH2cH2=O2+MEKenol2      3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
HO2+cH2C[O]C2H5=O2+MEKenol2   1.75E10     0.0   -3275.
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/OneDe

!MEKenol rxns: H-Abstractions
MEKenol+H=CH2C[OH]cHCH3+H2          1299000.0   2.38  2800.
      !H_Abstraction exact:   C/H3/Cd     H_rad
CH3C[OH]cCH3+H2=MEKenol+H           3.01E12     0.0   10600.
      !H_Abstraction exact:   Cd_rad/NonDeC     H2
MEKenol+H=CH3C[OH]CHcH2+H2          1299000.0   2.38  2800.
      !H_Abstraction exact:   C/H3/Cd     H_rad
MEKenol+H=CH3C[O]cHCH3+H2           1.3E11      0.82  7750.
      !H_Abstraction exact:   O/H/OneDe     H_rad
MEKenol+OH=CH2C[OH]cHCH3+H2O        3.448E7     1.75  3789.37
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
MEKenol+OH=CH3C[OH]cCH3+H2O         1110000.0   2.0   1450.
      !H_Abstraction exact:   Cd/H/NonDeC     O_pri_rad
MEKenol+OH=CH3C[OH]CHcH2+H2O        3.448E7     1.75  3789.37
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
MEKenol+OH=CH3C[O]cHCH3+H2O         17.3        3.4   -1140.
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_pri_rad
MEKenol+CH3=CH2C[OH]cHCH3+CH4       241.2       2.92  7160.
      !H_Abstraction exact:   C/H3/Cd     C_methyl
CH3C[OH]cCH3+CH4=MEKenol+CH3        1.590E14    0.0   13700.
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C_methane
MEKenol+CH3=CH3C[OH]CHcH2+CH4       241.2       2.92  7160.
      !H_Abstraction exact:   C/H3/Cd     C_methyl
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MEKenol+CH3=CH3C[O]cHCH3+CH4        90700.0     2.04  10850.
      !H_Abstraction exact:   O/H/OneDe     C_methyl
MEKenol+C2H3=CH2C[OH]cHCH3+C2H4     2.319E13    0.0   7500.
      !H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
MEKenol+C2H3=CH3C[OH]cCH3+C2H4      0.842       3.5   9670.
      !H_Abstraction exact:   Cd/H/NonDeC     Cd_pri_rad
MEKenol+C2H3=CH3C[OH]CHcH2+C2H4     2.319E13    0.0   7500.
      !H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
MEKenol+C2H3=CH3C[O]cHCH3+C2H4      14.40       3.1   6940.
      !H_Abstraction estimate: (Average:) O/H/OneDe     Cd_pri_rad
MEKenol+C2H5=CH2C[OH]cHCH3+C2H6     1.68E12     0.0   12400.
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
CH3C[OH]cCH3+C2H6=MEKenol+C2H5      5.036E12    0.0   9175.
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C/H3/Cs
MEKenol+C2H5=CH3C[OH]CHcH2+C2H6     1.68E12     0.0   12400.
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
MEKenol+C2H5=CH3C[O]cHCH3+C2H6      1486.7      2.386 9690.
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/Cs
MEKenol+aC3H5=CH2C[OH]cHCH3+C3H6    1.734E13    0.0   21400.
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
CH3C[OH]cCH3+C3H6=MEKenol+aC3H5     5.52E12     0.0   7500.
      !H_Abstraction exact:   Cd_rad/NonDeC     C/H3/Cd
MEKenol+aC3H5=CH3C[OH]CHcH2+C3H6    1.734E13    0.0   21400.
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
MEKenol+aC3H5=CH3C[O]cHCH3+C3H6     1486.7      2.386 9690.
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/Cd
!MEKenol rxns: Beta-scissions
!MEKenol+H=CH3CH[OH]CHCH3     1.0E13      0.0   2900.
      !R_Addition_MultipleBond estimate: (Average:)   Cd/Nd2_Cd/H/Nd
H_rad
!MEKenol+H=CH3C[OH]C2H5       1.0E13      0.0   2900.
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/Nd2
H_rad
!MEKenol rxns: R-Recombinations
!CH3+CH3CHcOH=MEKenol   1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    C_methyl     Cd_rad/NonDe
!CH2C[OH]cHCH3+H=MEKenol      5.00E13     0.0   0.0   !R_Recombination
estimate: (Average:)    C_rad/H2/Cd     H_rad
!C4H7-22+OH=MEKenol     1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     O_pri_rad
!CH3C[OH]cH+CH3=MEKenol 7.23E13     0.0   0.0   !R_Recombination exact:
      Cd_pri_rad     C_methyl
!CH3C[OH]cCH3+H=MEKenol 1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     H_rad
!CH3C[OH]CHcH2+H=MEKenol      5.00E13     0.0   0.0   !R_Recombination
estimate: (Average:)    C_rad/H2/Cd     H_rad
!CH3C[O]cHCH3+H=MEKenol 1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    O_rad/OneDe     H_rad
!MEKenol rxns: Disproportionations
HO2+CH2C[OH]cHCH3=O2+MEKenol  3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cd
HO2+CH3C[OH]cCH3=O2+MEKenol   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     Cd_rad/NonDeC
HO2+CH3C[OH]CHcH2=O2+MEKenol  3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cd
HO2+CH3C[O]cHCH3=O2+MEKenol   1.75E10     0.0   -3275.
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/OneDe
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!sC4H8O rxns: H-Abstractions
cH2CH[OH]C2H3+H2=sC4H8O+H           4.57E11     0.0   14800.
      !H_Abstraction exact:   C_rad/H2/Cs     H2
sC4H8O+H=CH3C[OH]CHcH2+H2           3020000.0   2.16  -450.
      !H_Abstraction estimate: (Average:) C/H/ODMustO     H_rad
CH3CH[OH]cCH2+H2=sC4H8O+H           3.01E12     0.0   10600.
      !H_Abstraction exact:   Cd_rad/NonDeC     H2
CH3CH[OH]CHcH+H2=sC4H8O+H           4.49E12     0.0   10300.
      !H_Abstraction exact:   Cd_pri_rad     H2
CH3CH[o]C2H3+H2=sC4H8O+H            0.0632      4.0   4910.
      !H_Abstraction exact:   O_rad/NonDeC     H2
sC4H8O+OH=cH2CH[OH]C2H3+H2O         3600000.0   2.0   860.
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
sC4H8O+OH=CH3C[OH]CHcH2+H2O         6.56E8      0.95  3997.75
      !H_Abstraction estimate: (Average:) C/H/ODMustO     O_pri_rad
sC4H8O+OH=CH3CH[OH]cCH2+H2O         1110000.0   2.0   1450.
      !H_Abstraction exact:   Cd/H/NonDeC     O_pri_rad
sC4H8O+OH=CH3CH[OH]CHcH+H2O         1.026E13    0.0   5940.
      !H_Abstraction exact:   Cd_pri     O_pri_rad
sC4H8O+OH=CH3CH[o]C2H3+H2O          17.3        3.4   -1140.
      !H_Abstraction exact:   O/H/NonDeC     O_pri_rad
sC4H8O+CH3=cH2CH[OH]C2H3+CH4        834000.0    1.9   11050.
      !H_Abstraction exact:   C/H3/Cs     C_methyl
sC4H8O+CH3=CH3C[OH]CHcH2+CH4        2.73E13     0.0   8900.
      !H_Abstraction estimate: (Average:) C/H/ODMustO     C_methyl
CH3CH[OH]cCH2+CH4=sC4H8O+CH3        1.59E14     0.0   13700.
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C_methane
CH3CH[OH]CHcH+CH4=sC4H8O+CH3        1.59E14     0.0   13700.
      !H_Abstraction exact:   Cd_pri_rad     C_methane
CH3CH[o]C2H3+CH4=sC4H8O+CH3         1.55E-4     5.0   5580.
      !H_Abstraction exact:   O_rad/NonDeC     C_methane
sC4H8O+C2H3=cH2CH[OH]C2H3+C2H4      1.511E13    0.0   9175.
      !H_Abstraction estimate: (Average:) C/H3/Cs     Cd_pri_rad
sC4H8O+C2H3=CH3C[OH]CHcH2+C2H4      7.635E12    0.0   7725.
      !H_Abstraction estimate: (Average:) C/H/ODMustO     Cd_pri_rad
sC4H8O+C2H3=CH3CH[OH]cCH2+C2H4      0.842       3.5   9670.
      !H_Abstraction exact:   Cd/H/NonDeC     Cd_pri_rad
CH3CH[OH]CHcH+C2H4=sC4H8O+C2H3      1.47E13     0.0   13100.
      !H_Abstraction exact:   Cd_pri_rad     Cd_pri
sC4H8O+C2H3=CH3CH[o]C2H3+C2H4 14.4        3.1   6940.
      !H_Abstraction exact:   O/H/NonDeC     Cd_pri_rad
cH2CH[OH]C2H3+C2H6=sC4H8O+C2H5      659.0       2.71  12920.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
sC4H8O+C2H5=CH3C[OH]CHcH2+C2H6      1.621E9     1.004 11128.6
      !H_Abstraction estimate: (Average:) C/H/ODMustO     C_rad/H2/Cs
CH3CH[OH]cCH2+C2H6=sC4H8O+C2H5      5.036E12    0.0   9175.
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C/H3/Cs
CH3CH[OH]CHcH+C2H6=sC4H8O+C2H5      5.036E12    0.0   9175.
      !H_Abstraction estimate: (Average:) Cd_pri_rad     C/H3/Cs
CH3CH[o]C2H3+C2H6=sC4H8O+C2H5 4.74E11     0.0   7000.
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
cH2CH[OH]C2H3+C3H6=sC4H8O+aC3H5     5.6E11      0.0   12400.
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
sC4H8O+aC3H5=CH3C[OH]CHcH2+C3H6     1.621E9     1.004 11128.6
      !H_Abstraction estimate: (Average:) C/H/ODMustO     C_rad/H2/Cd
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CH3CH[OH]cCH2+C3H6=sC4H8O+aC3H5     5.52E12     0.0   7500.
      !H_Abstraction exact:   Cd_rad/NonDeC     C/H3/Cd
CH3CH[OH]CHcH+C3H6=sC4H8O+aC3H5     7.73E12     0.0   7500.
      !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
CH3CH[o]C2H3+C3H6=sC4H8O+aC3H5      1.149E7     1.75  3789.37
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/Cd
!sC4H8O rxns: Beta-scissions
!sC4H8O+H=CH3CH[OH]CH2CH2     1.18E13     0.0   3800.
      !R_Addition_MultipleBond exact:     Cd/H/Nd_Cd/H2     H_rad
!sC4H8O+H=CH3CH[OH]CHCH3      2.01E13     0.0   2100.
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/Nd     H_rad
!sC4H8O rxns: R-Recombinations
!CH3+C3H5O-enol2=sC4H8O 6.80E14     -0.68 0.0   !R_Recombination
estimate: (Average:)    C_methyl     C_rad/H/OneDeO
!cH2CH[OH]C2H3+H=sC4H8O 1.0E14      0.0   0.0   !R_Recombination exact:
      C_rad/H2/Cs     H_rad
!C2H5O-2+C2H3=sC4H8O    1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    C_rad/H/CsO     Cd_pri_rad
!C4H7-24+OH=sC4H8O      1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    C_rad/H/OneDeC     O_pri_rad
!CH3C[OH]CHcH2+H=sC4H8O 5.0E13      0.0   0.0   !R_Recombination
estimate: (Average:)    C_rad/ODMustO     H_rad
!CH3CH[OH]cCH2+H=sC4H8O 1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    Cd_rad/NonDe     H_rad
!CH3CH[OH]CHcH+H=sC4H8O 5.36E14     0.0   980.  !R_Recombination exact:
      Cd_pri_rad     H_rad
!CH3CH[o]C2H3+H=sC4H8O  1.416E13    -0.15 291.7 !R_Recombination
estimate: (Average:)    O_rad/NonDe     H_rad
!sC4H8O rxns: Disproportionations
HO2+cH2CH[OH]C2H3=O2+sC4H8O   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
HO2+CH3C[OH]CHcH2=O2+sC4H8O   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/ODMustO
HO2+CH3CH[OH]cCH2=O2+sC4H8O   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     Cd_rad/NonDeC
HO2+CH3CH[OH]CHcH=O2+sC4H8O   3.00E11     0.0   0.0
      !Disproportionation estimate: (Average:)  O_Orad     Cd_pri_rad
HO2+CH3CH[o]C2H3=O2+sC4H8O    1.75E10     0.0   -3275.
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/NonDeC

!C4H7O radical rxns
!CH2CO+C2H5=cH2C[O]C2H5 1.93E11     0.04  9290.0
      !R_Addition_MultipleBond estimate: (Average:)   Ck_Cd/H2
C_rad/H2/Cs
!C4H7-12+O=cH2C[O]C2H5  1.00E13     0.0   0.0
      !Oa_R_Recombination estimate: (Average:)  Cd_rad/NonDe     Oa

!CH3+C3H4O-enone=CH3C[O]cHCH3 2.815E12    0.0   7856.67
      !R_Addition_MultipleBond estimate: (Average:)   C_methyl
Ck_Cd/H/Nd
!C4H6O(60)+H=CH3C[O]cHCH3     3.71E13     0.0   1000.
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/De     H_rad
!C4H7-22+O=CH3C[O]cHCH3       1.000E13    0.0   0.0
      !Oa_R_Recombination estimate: (Average:)  Cd_rad/NonDe     Oa
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!CH3CO+C2H4=CH3C[O]CH2cH2     5.2011      0.0   6560.
      !R_Addition_MultipleBond estimate: (Average:)   CO_rad/NonDe
Cd/H2_Cd/H2
!C4H6O(60)+H=CH3C[O]CH2cH2          2.85E13     0.0   4300.
      !R_Addition_MultipleBond exact:     Cd/H/De_Cd/H2     H_rad
!C3H7-1+CO=CH3C[O]CH2cH2            538.0       3.29  104500.
      !1,2_Insertion exact:   Cs_Cs     CO_birad

!C4H6-12+OH=CH2C[OH]cHCH3     2.74E10     0.57  3788.89
      !R_Addition_MultipleBond estimate: (Average:)   Ca_Cd/H/Nd
O_pri_rad
!C4H6O(16)+H=CH2C[OH]cHCH3    3.71E13     0.0   1000.
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/De     H_rad

!C2H3O-2+C2H4=CH2C[OH]CH2cH2  7.24E12     0.0   4500.
      !R_Addition_MultipleBond exact:     Cd_rad/NonDe     Cd/H2_Cd/H2
!C4H6O(10)+H=CH2C[OH]CH2cH2   2.85E13     0.0   4300.
      !R_Addition_MultipleBond exact:     Cd/H/De_Cd/H2     H_rad

!HCCOH+C2H5=cHC[OH]C2H5 2.00E10     0.0   6975. !R_Addition_MultipleBond
estimate: (Average:)    Ct/Nd_Ct/H     C_rad/H2/Cs
!C4H6-1+OH=cHC[OH]C2H5  7.60E7      1.7   1000. !R_Addition_MultipleBond
estimate: (Average:)    Ct/Nd_Ct/H     O_pri_rad

!CH3+C3H4O(7)=CH3C[OH]cCH3    2.245E13    0.0   10220.
      !R_Addition_MultipleBond estimate: (Average:)   C_methyl
Ct/Nd_Ct/Nd
!C4H6-2+OH=CH3C[OH]cCH3       7.60E7      1.7   1000.
      !R_Addition_MultipleBond estimate: (Average:)   Ct/Nd_Ct/Nd
O_pri_rad
!C4H6O(10)+H=CH3C[OH]cCH3     6.68E13     0.0   2900.
      !R_Addition_MultipleBond exact:     Cd/H2_Ca     H_rad

!C4H6O(14)+H=CH3C[OH]CHcH2    1.2E11      0.69  3000.
      !R_Addition_MultipleBond exact:     Ca_Cd/H2     H_rad
!C4H6O(16)+H=CH3C[OH]CHcH2    7.299E11    0.18  2985.1
      !R_Addition_MultipleBond estimate: (Average:)   OCO     H_rad
!C4H6O(17)+H=CH3C[OH]CHcH2    2.13E13     0.0   500.
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/Nd/De     H_rad

!CH3+HCCOH=CH3C[OH]cH   1.99E13     0.0   12100.
      !R_Addition_MultipleBond exact:     C_methyl     Ct/Nd_Ct/H
!pC3H4+OH=CH3C[OH]cH    7.60E7      1.7   1000.
      !R_Addition_MultipleBond estimate: (Average:)   Ct/Nd_Ct/H
O_pri_rad

HCCOH+CH3=CH3CHcOH      1.32E14     0.0   10300.
      !R_Addition_MultipleBond exact:     Ct/H_Ct/Nd     C_methyl
!C3H4O(8)+H=CH3CHcOH    5.00E13     0.0   4100.
      !R_Addition_MultipleBond estimate: (Average:)   Ct/Nd_Ct/Nd
H_rad

!C2H4O+C2H3=cH2CH[OH]C2H3     149.03      3.0   10170.8
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/H2
Cd_pri_rad
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!C4H6-13+OH=cH2CH[OH]C2H3     2.71E12     0.0   0.0
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/De_Cd/H2
O_pri_rad
!C4H6O(13)+H=cH2CH[OH]C2H3    9.3E12      0.0   5200.
      !R_Addition_MultipleBond exact:     Cd/Nd/De_Cd/H2     H_rad

!CH3+C3H4O(8)=CH3CH[OH]cCH2   8.857E11    0.0   10000.
      !R_Addition_MultipleBond estimate: (Average:)   C_methyl
Cd/H/Nd_Ca
!C4H6-12+OH=CH3CH[OH]cCH2     2.74E10     0.57  3788.89
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Ca
O_pri_rad
!C4H6O(11)+H=CH3CH[OH]cCH2    1.0E13      0.0   2900.
      !R_Addition_MultipleBond exact:     Cd/Nd2_Ca     H_rad
!C4H6O(13)+H=CH3CH[OH]cCH2    1.12E14     0.0   3700.
      !R_Addition_MultipleBond exact:     Ct/H_Ct/Nd     H_rad

!C2H5O-2+C2H2=CH3CH[OH]CHcH   2.505E10    0.0   6900.
      !R_Addition_MultipleBond estimate: (Average:)   C_rad/H/CsO
Ct/H_Ct/H
!C4H6O(9)+H=CH3CH[OH]CHcH     5.77E13     0.0   5300.
      !R_Addition_MultipleBond exact:     Ct/Nd_Ct/H     H_rad

!CH3+C3H4O=CH3CH[o]C2H3       3.16E10     0.0   11510.
      !R_Addition_MultipleBond estimate: (Average:)   C_methyl
CO/H/De_O
!CH3CHO+C2H3=CH3CH[o]C2H3     3.28E7      1.50  7335.4
      !R_Addition_MultipleBond estimate: (Average:)   CO/H/Nd_O
Cd_pri_rad
!C4H6O(13)+H=CH3CH[o]C2H3     1.00E11     0.0   11900.
      !R_Addition_MultipleBond estimate: (Average:)   CO/Nd/De_O
H_rad

CH2O+pC3H3=HCO+pC3H4    5500.0      2.81  5860.0      !H_Abstraction
estimate: (Average:)    CO_pri     C_rad/H2/Ct
HCO+aC3H4=CH2O+pC3H3    5.589E9     0.976 15188.25    !H_Abstraction
estimate: (Average:)    CO_pri_rad     Cd_pri

nC4H8O+O=C4H7OJ(16)+OH  25650.0     3.05  3.123e3     !H_Abstraction
exact:      C/H3/Cs     O_atom_triplet
nC4H8O+O=C4H7OJ(13)+OH  47800.0     2.71  2.11e3      !H_Abstraction
exact:      C/H2/NonDeC     O_atom_triplet
nC4H8O+O=C4H7OJ(12)+OH  47800.0     2.71  2.11e3      !H_Abstraction
estimate: (Average:)    C/H2/OneDeC     O_atom_triplet

!Pressure-dependent networks
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!
! CH2O2 PES for n-butanol:
!    *C-O-*O   *O-C-*O   O-O
!                        \ /
!                         C
! Method: ReservoirState
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!

!sSPC(2810)+H(+m)=CH2+O2(+m)  1.0E0 0.0 0.0     !No comment
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!TCHEB / 300.0 2100.0 / PCHEB / 0.01 100.0 /
!CHEB / 4   4 /
!CHEB / -2.4750000e+01 -6.9139000e+00 5.9261000e+00 -3.4570000e+00 /
!CHEB / 2.1256000e+01 7.3760000e+00 -6.3220000e+00 3.6880000e+00 /
!CHEB / -2.1230000e-02 -4.0121000e-02 3.4244000e-02 -2.0062000e-02 /
!CHEB / 1.2369000e-01 -2.1212000e-01 1.8179000e-01 -1.0606000e-01 /

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!
! New work for sec- and tert-butanol paper:
!
!    "Accurate Reaction Networks for Alternative Fuels: Butanol Isomers"
!
!    K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
!
!    To be submitted to Industrial & Engineering Chemical Research
!
!       for the ISCRE-21 conference
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!

! Following reaction rate expressions from:
!    Kislov, V.V.; Mebel, A.M.; J. Phys. Chem. A v.111 (2007) 3922-3931
!    MRH fit the k(T) data to a modified Arrhenius expression, using
least-squares regression
benzene+CH3=CH4+C6H5    4.919e+03   2.902 15299.0
C7H8+H=C7H9             2.734e+06   1.768 5814.0

!Following reaction rate expression from:
!    Seta, T.; Nakajima, M.; Miyoshi, A.; J. Phys. Chem. A v.110 (2006)
5081-5090
C7H8+OH=H2O+C6H5CH2     1.81e+05    2.39  -602.29

!Following reaction rate expressions from:
!    RMG
C7H8+CH3=CH4+C6H5CH2    4.90E+12    0.0   13.1e+03    !H_Abstraction:
C/H3/Cb   C_methyl
C2H5O-2+O2=HO2+C2H4O    7.56E+11    0.0   0.0   !Disproportionation_O2d
exact:      O2d     Cmethyl_Csrad
!C2H5O-2+O2=HO2+CH3CHO  2.28E+13    0.0   0.0   !Disproportionation_O2d
exact:      O2d     O_Csrad
C2H5O-2+O2=HO2+CH3CHO   4.6826e+11 0.3321 -1.0635e+03 !from rate
calculated by Zador et al (consistent with RMG) edited by MRH 05.12.11
sBuOH+nC4H5=CH2CH[OH]C2H5+C4H6-13   1.511E13    0.0   9.175e+03
      !H_Abstraction estimate: (Average:) C/H3/Cs     Cd_pri_rad
sBuOH+nC4H5=CH3C[OH]C2H5+C4H6-13    8.950E13    0.0   6.2e+03
      !H_Abstraction estimate: (Average:) C/H/NDMustO     Cd_pri_rad
sBuOH+nC4H5=CH3CH[OH]CHCH3+C4H6-13  1020.0      3.1   8.82e+03
      !H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
sBuOH+nC4H5=CH3CH[OH]CH2CH2+C4H6-13 1.511E13    0.0   9.175e+03
      !H_Abstraction estimate: (Average:) C/H3/Cs     Cd_pri_rad
sBuOH+nC4H5=CH3CH[O]C2H5+C4H6-13    14.4        3.1   6.94e+03
      !H_Abstraction exact:   O/H/NonDeC     Cd_pri_rad
CH2CH[OH]C2H5+C4H6-13=sBuOH+iC4H5   5.060E12    0.0   16.25e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     Cd/H/OneDe
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sBuOH+iC4H5=CH3C[OH]C2H5+C4H6-13    6.514E11    0.0   9.25e+03
      !H_Abstraction estimate: (Average:) C/H/NDMustO     Cd_rad/OneDe
sBuOH+iC4H5=CH3CH[OH]CHCH3+C4H6-13  1020.0      3.1   8.82e+03
      !H_Abstraction estimate: (Average:) C/H2/NonDeC     Cd_rad/OneDe
CH3CH[OH]CH2CH2+C4H6-13=sBuOH+iC4H5 5.060E12    0.0   16.25e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     Cd/H/OneDe
CH3CH[O]C2H5+C4H6-13=sBuOH+iC4H5    1110000.0   2.0   1.45e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     Cd/H/OneDe
nC4H5+aC3H5=C4H6-13+aC3H4           2.41E12     0.0   0.0e+03
      !Disproportionation exact:    Cd_pri_rad     Cdpri_Csrad
iC4H5+aC3H5=C4H6-13+aC3H4           2.41E12     0.0   0.0e+03
      !Disproportionation estimate: (Average:)  Cd_rad/OneDe
Cdpri_Csrad
iC4H5+aC3H5=C4H6-12+aC3H4           8.43E10     0.0   -0.26e+03
      !Disproportionation exact:    Cdpri_Csrad     C_rad/H2/Cd
C2H+C4H7-24=C2H2+C4H6-12            5.413E12    -0.08875    -
0.0365625e+03     !Disproportionation estimate: (Average:)  Ct_rad
Cdpri_Csrad
C2H+C4H7-24=C2H2+C4H6-13            1.083E13    0.0   0.0e+03
      !Disproportionation exact:    Ct_rad     Cmethyl_Csrad
aC3H5+C4H7-24=C3H6+C4H6-12          8.43E10     0.0   -0.26e+03
      !Disproportionation exact:    C_rad/H2/Cd     Cdpri_Csrad
aC3H5+C4H7-24=C3H6+C4H6-13          6.87E13     -0.35 -0.13e+03
      !Disproportionation exact:    Cmethyl_Csrad     C_rad/H2/Cd
!C4H8-1+H=C4H7-24+H2                1.398e+06   2.36  1110.00
      !H_Abstraction exact:   C/H2/OneDeC     H_rad
!C4H8-1+CH3=C4H7-24+CH4                  5.460e+13   0.00  10400.00
      !H_Abstraction exact:   C/H2/OneDeC     C_methyl

!Following reaction rate expressions from:
!    TST w/Wigner tunneling correction
!    Energies computed at CBS-QB3 level; vibrations at B3LYP/CBSB7
!    1dHR corrections computed at B3LYP/6-31G(d)
sBuOH+H=H2+CH3C[OH]C2H5             4.14e+05    2.34   2.68e+03
sBuOH+H=H2+CH3CH[OH]CHCH3           8.65e+05    2.30   4.68e+03
sBuOH+H=H2+CH3CH[O]C2H5             5.01e+04    2.64   7.15e+03
sBuOH+H=H2+CH2CH[OH]C2H5            5.68e+06    2.21   7.50e+03
sBuOH+H=H2+CH3CH[OH]CH2CH2          1.68e+06    2.21   9.58e+03

sBuOH+CH3=CH4+CH3C[OH]C2H5          3.89e-01    3.53   4.01e+03
sBuOH+CH3=CH4+CH3CH[OH]CHCH3        1.21e+01    3.43   9.58e+03
sBuOH+CH3=CH4+CH3CH[O]C2H5          1.53e-02    3.92   7.89e+03
sBuOH+CH3=CH4+CH2CH[OH]C2H5         1.42e+00    3.60  11.05e+03
sBuOH+CH3=CH4+CH3CH[OH]CH2CH2       1.59e+00    3.62  13.43e+03


!!! tBuOH reactions
tBuOH+CH3=HOC[CH2][CH3]2+CH4 1.320e+01     3.40        11970.00
!Primary Reaction Library: MRH_tBuOH_rxns
tBuOH+CH3=OC[CH3]3+CH4 2.990e-01     3.73        10800.00    !Primary
Reaction Library: MRH_tBuOH_rxns
tBuOH+sC3H5=HOC[CH2][CH3]2+C3H6 1.320e+01        3.50        11970.00
!Primary Reaction Library: MRH_tBuOH_rxns
tBuOH+sC3H5=OC[CH3]3+C3H6 2.990e-01        3.73        8800.00
!Primary Reaction Library: MRH_tBuOH_rxns
iC4H8+sC3H5=iC4H7+C3H6 1.8240000e+02       2.92000     9160.00000
!H_Abstraction exact:   C/H3/Cd     C_methyl
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HCC[CH3]2+C3H6=iC4H8+sC3H5 1.5900000e+13   0.00000     13700.00000
!H_Abstraction exact:   Cd_pri_rad     C_methane
pC3H3+iC4H5=C7H8  1.5900000e+13      0.00000     0.00000
      !recombination kevin

OC[CH3]3+tBuOH=tBuOH+HOC[CH2][CH3]2 4.7400000e+11      0.00000
7000.00000   !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
HOC[CH2][CH3]2+CH3C[OH]CH3=tBuOH+acetone 2.4100000e+12       0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
OC[CH3]3+CH3C[OH]CH3=tBuOH+acetone 2.4100000e+13       0.00000
0.00000      !Disproportionation exact:   O_rad/NonDeC     O_Csrad
HOC[CH2][CH3]2+CH3C[OH]CH3=tBuOH+H2CCCH3[OH] 1.3800000e+14   -0.35000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
!OC[CH3]3+CH3C[OH]CH3=tBuOH+H2CCCH3[OH] 1.4460000e+14        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeC
Cmethyl_Csrad
OH+tBuOH=H2O+HOC[CH2][CH3]2 1.2000000e+06        2.00000     860.00000
!H_Abstraction exact:   O_pri_rad     C/H3/Cs
OH+tBuOH=H2O+OC[CH3]3 1.7300000e+01        3.40000     -1140.00000
!H_Abstraction exact:   O_pri_rad     O/H/NonDeC
tBuOH+H=OC[CH3]3+H2 9.590e+04        2.56        10710.00    !Primary
Reaction Library: MRH_tBuOH_rxns
tBuOH+H=HOC[CH2][CH3]2+H2 7.860e+06        2.30        9430.00
!Primary Reaction Library: MRH_tBuOH_rxns
!tBuOH+H=HOC[CH2][CH3]2+H2 5.6520000e+08   1.75000     7510.00000
!H_Abstraction exact:   C/H3/Cs     H_rad
!iC4H8+CH3=iC4H7+CH4 2.8240000e+02   4.92000     9160.00000
!H_Abstraction exact:   C/H3/Cd     C_methyl
!iC4H8+HOC[CH2][CH3]2=iC4H7+tBuOH 3.3600000e+12        0.00000
12400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
iC4H8+HOC[CH2][CH3]2=iC4H7+tBuOH    2.23  3.5   6.64e+03
      !C3H6+iC4H9=iC4H10+aC3H5 (Tsang)
iC4H8+OC[CH3]3=iC4H7+tBuOH 6.8964034e+07   1.75000     5789.37500
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_rad/NonDeC
CH3C[OH]CH3+iC4H7=acetone+iC4H8 1.8100000e+13    0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cd
!CH3C[OH]CH3+iC4H7=H2CCCH3[OH]+iC4H8 2.2900000e+13     -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
!iC4H8+H=iC4H7+H2 2.5980000e+06      2.38000     2800.00000
!H_Abstraction exact:   C/H3/Cd     H_rad
iC4H8+OH=iC4H7+H2O 6.8964034e+07     1.75000     3789.37500
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_pri_rad
CH2C[O]CH3+tBuOH=acetone+HOC[CH2][CH3]2 6.5900000e+02        2.71000
12920.00000        !H_Abstraction estimate: (Average:)  C_rad/H2/CO
C/H3/Cs
acetone+OC[CH3]3=CH2C[O]CH3+tBuOH 6.8964034e+07        1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/CO
O_rad/NonDeC
H2CCCH3[OH]+HOC[CH2][CH3]2=CH2C[O]CH3+tBuOH 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
H2CCCH3[OH]+OC[CH3]3=CH2C[O]CH3+tBuOH 1.7300000e+01    3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeC
!CH2C[O]CH3+iC4H8=acetone+iC4H7 2.9057730e+12    0.00000     17333.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/CO     C/H3/Cd
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CH2C[O]CH3+iC4H8=H2CCCH3[OH]+iC4H7 1.1494006e+06       1.75000
10789.37500        !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H3/Cd
H2CCCH3[OH]+HOC[CH2][CH3]2=CH2C[OH]CH2+tBuOH 1.6800000e+12   0.00000
12400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
H2CCCH3[OH]+OC[CH3]3=CH2C[OH]CH2+tBuOH 3.4482017e+07   1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeC
CH2C[OH]CH2+iC4H8=H2CCCH3[OH]+iC4H7 5.7800000e+12      0.00000
21400.00000        !H_Abstraction exact:   C_rad/H2/Cd     C/H3/Cd
HCC[CH3]2+CH4=iC4H8+CH3 1.5900000e+13      0.00000     13700.00000
!H_Abstraction exact:   Cd_pri_rad     C_methane
HCC[CH3]2+tBuOH=iC4H8+HOC[CH2][CH3]2 5.0359704e+12     0.00000
9175.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
HCC[CH3]2+tBuOH=iC4H8+OC[CH3]3 1.4400000e+01     3.10000     6940.00000
       !H_Abstraction exact:   Cd_pri_rad     O/H/NonDeC
CH3C[OH]CH3+HCC[CH3]2=acetone+iC4H8 3.0100000e+13      0.00000
0.00000      !Disproportionation exact:   O_Csrad     Cd_pri_rad
CH3C[OH]CH3+HCC[CH3]2=H2CCCH3[OH]+iC4H8 1.5200000e+14        -0.70000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
HCC[CH3]2+H2=iC4H8+H 4.4900000e+12   0.00000     10300.00000
!H_Abstraction exact:   Cd_pri_rad     H2
iC4H8+OH=HCC[CH3]2+H2O 1.0260000e+13       0.00000     5940.00000
!H_Abstraction exact:   Cd_pri     O_pri_rad
HCC[CH3]2+iC4H8=iC4H8+iC4H7 7.7300000e+12        0.00000     7500.00000
       !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
HCC[CH3]2+acetone=iC4H8+CH2C[O]CH3 5.0359704e+12       0.00000
9175.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/CO
HCC[CH3]2+H2CCCH3[OH]=iC4H8+CH2C[O]CH3 1.4400000e+01   3.10000
6940.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad
O/H/OneDe
HCC[CH3]2+H2CCCH3[OH]=iC4H8+CH2C[OH]CH2 7.7300000e+12        0.00000
7500.00000   !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
CH3C[OH]cH+CH4=H2CCCH3[OH]+CH3 1.5900000e+14     0.00000     13700.00000
       !H_Abstraction exact:   Cd_pri_rad     C_methane
CH3C[OH]cH+tBuOH=H2CCCH3[OH]+HOC[CH2][CH3]2 5.0359704e+12    0.00000
9175.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/Cs
CH3C[OH]cH+tBuOH=H2CCCH3[OH]+OC[CH3]3 1.4400000e+01    3.10000
6940.00000   !H_Abstraction exact:   Cd_pri_rad     O/H/NonDeC
CH3C[OH]CH3+CH3C[OH]cH=acetone+H2CCCH3[OH] 3.0100000e+13     0.00000
0.00000      !Disproportionation exact:   O_Csrad     Cd_pri_rad
CH3C[OH]cH+H2=H2CCCH3[OH]+H 4.4900000e+12        0.00000     10300.00000
       !H_Abstraction exact:   Cd_pri_rad     H2
H2CCCH3[OH]+OH=CH3C[OH]cH+H2O 1.0260000e+12      0.00000     9940.00000
       !H_Abstraction exact:   Cd_pri     O_pri_rad
CH3C[OH]cH+iC4H8=H2CCCH3[OH]+iC4H7 7.7300000e+12       0.00000
7500.00000   !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
CH3C[OH]cH+acetone=H2CCCH3[OH]+CH2C[O]CH3 5.0359704e+12      0.00000
9175.00000   !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H3/CO
CH3C[OH]cH+H2CCCH3[OH]=H2CCCH3[OH]+CH2C[O]CH3 1.4400000e+01
3.10000      6940.00000        !H_Abstraction estimate: (Average:)
Cd_pri_rad     O/H/OneDe
CH3C[OH]cH+H2CCCH3[OH]=H2CCCH3[OH]+CH2C[OH]CH2 7.7300000e+12
0.00000      7500.00000        !H_Abstraction exact:   Cd_pri_rad
C/H3/Cd
CH3C[OH]cH+iC4H8=H2CCCH3[OH]+HCC[CH3]2 1.4700000e+13   0.00000
13100.00000        !H_Abstraction exact:   Cd_pri_rad     Cd_pri
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!!!!!!!!!!!!!
iC4H9+tC4H9=iC4H10+iC4H8      2.07E14     -0.35 0.0e+03
      !Disproportionation exact:    C_rad/H2/Cs     Cmethyl_Csrad
iC4H9+iC4H9=iC4H10+iC4H8      8.43E11     0.0   0.0e+03
      !Disproportionation exact:    C_rad/H2/Cs     C/H/NdNd_Csrad
tC4H9+tC4H9=iC4H10+iC4H8      2.574E16    -1.1  0.0e+03
      !Disproportionation exact:    C_rad/Cs3     Cmethyl_Csrad

OC[CH3]3+iC4H10=tBuOH+tC4H9         2.29E10     0.0   2.88e+03
      !H_Abstraction exact:   O_rad/NonDeC     C/H/Cs3
HOC[CH2][CH3]2+iC4H10=tBuOH+tC4H9   4220.0      2.51  8.06e+03
      !H_Abstraction exact:   C_rad/H2/Cs     C/H/Cs3
OC[CH3]3+iC4H10=tBuOH+iC4H9         4.74E11     0.0   7.0e+03
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
HOC[CH2][CH3]2+iC4H10=tBuOH+iC4H9   659.0       2.71  12.92e+03
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
CH3+iC4H10=CH4+tC4H9                574000.0    1.83  6.94e+03
      !H_Abstraction exact:   C_methyl     C/H/Cs3
CH3+iC4H10=CH4+iC4H9                278000.0    1.9   11.05e+03
      !H_Abstraction exact:   C_methyl     C/H3/Cs

!pC3H3 reactions w/Butanols
CH2CH[OH]C2H5+pC3H4=sBuOH+pC3H3     9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H3/Ct
CH3C[OH]C2H5+pC3H4=sBuOH+pC3H3      9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/NDMustO     C/H3/Ct
CH3CH[OH]CHCH3+pC3H4=sBuOH+pC3H3    9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H3/Ct
CH3CH[OH]CH2CH2+pC3H4=sBuOH+pC3H3   9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H3/Ct
CH3CH[O]C2H5+pC3H4=sBuOH+pC3H3      3.448E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/Ct
OC[CH3]3+pC3H4=tBuOH+pC3H3          3.448E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/Ct
HOC[CH2][CH3]2+pC3H4=tBuOH+pC3H3    9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H3/Ct
C4H9O-1+pC3H4=nC4H10O+pC3H3         9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H3/Ct
C4H9O-2+pC3H4=nC4H10O+pC3H3         9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H3/Ct
C4H9O-3+pC3H4=nC4H10O+pC3H3         9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H3/Ct
C4H9O-4+pC3H4=nC4H10O+pC3H3         9.407E+06   1.753 12.53e+03
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H3/Ct
C4H9O-5+pC3H4=nC4H10O+pC3H3         3.448E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/Ct
CH2CH[OH]C2H5+aC3H4=sBuOH+pC3H3     3.128E13    0.0   19.7e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H2/Cs
CH3C[OH]C2H5+aC3H4=sBuOH+pC3H3      1.572E14    0.0   20.1e+03
      !H_Abstraction estimate: (Average:) C_rad/NDMustO     Cd_pri
CH3CH[OH]CHCH3+aC3H4=sBuOH+pC3H3    1.3E13      0.0   20.2e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H/NonDeC
CH3CH[OH]CH2CH2+aC3H4=sBuOH+pC3H3   3.128E13    0.0   19.7e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H2/Cs
CH3CH[O]C2H5+aC3H4=sBuOH+pC3H3      2.052E13    0.0   5.94e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     Cd_pri
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OC[CH3]3+aC3H4=tBuOH+pC3H3          2.052E13    0.0   5.94e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     Cd_pri
HOC[CH2][CH3]2+aC3H4=tBuOH+pC3H3    3.128E13    0.0   19.7e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H2/Cs
C4H9O-1+aC3H4=nC4H10O+pC3H3         3.128E13    0.0   19.7e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H2/Cs
C4H9O-2+aC3H4=nC4H10O+pC3H3         1.3E13      0.0   20.2e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H/NonDeC
C4H9O-3+aC3H4=nC4H10O+pC3H3         1.3E13      0.0   20.2e+03
      !H_Abstraction exact:   Cd_pri     C_rad/H/NonDeC
C4H9O-4+aC3H4=nC4H10O+pC3H3         2.80213     0.0   25.95e+03
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     Cd_pri
C4H9O-5+aC3H4=nC4H10O+pC3H3         2.052E13    0.0   5.94e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     Cd_pri

!Replaced Marinov values with RMG values
pC3H4+OH=pC3H3+H2O      3.448E7     1.75  3.789e+03   !H_Abstraction
estimate: (Average:)    C/H3/Ct     O_pri_rad
aC3H4+OH=pC3H3+H2O      2.052E13    0.0   5.94e+03    !H_Abstraction
exact:      Cd_pri     O_pri_rad
!aC3H4+H=pC3H3+H2       1.012E8     1.98  11.78e+03   !H_Abstraction
exact:      Cd_pri     H_rad

!Replaced RMG value with value recommended by Tsang (t-
C4H9+O2=HO2+iC4H8)
C5H4CH3+O2=HO2+FULVENE  4.82E+11    0.0   0.0

!Replaced RMG values w/MRH CBS-QB3 calculations
H+C4H8-1=C4H7-24+H2     4.50e+04    2.67  3.48e+03
H+C4H8-2=C4H7-24+H2     6.70e+03    3.14  4.29e+03
H+iC4H8=iC4H7+H2        5.03e+03    3.18  4.37e+03
CH3+C4H8-1=C4H7-24+CH4  2.04e-01    3.99  6.27e+03
CH3+C4H8-2=C4H7-24+CH4  1.45e-01    4.25  7.53e+03
CH3+iC4H8=iC4H7+CH4     1.19e-01    4.26  7.55e+03

iC4H10+H=iC4H9+H2       5.652E8     1.75  7.51e+03    !H_Abstraction
exact:      C/H3/Cs     H_rad
iC4H10+H=tC4H9+H2       4.83E8      1.54  2.98e+03    !H_Abstraction
exact:      C/H/Cs3     H_rad
iC4H10+OH=iC4H9+H2O     1.08E7      2.0   0.86e+03    !H_Abstraction
exact:      C/H3/Cs     O_pri_rad
iC4H10+OH=tC4H9+H2O     1700000.0   1.9   -1.451e+03  !H_Abstraction
exact:      C/H/Cs3     O_pri_rad


!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! s-butanol oxidation chemistry !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!C4H8-1+HO2=C4H7-24+H2O2 3.1729268e+09     0.95000     5644.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     O_rad/NonDeO
HO2+CH3CH[OH]CHCH3=O2+sBuOH 3.0000000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     C_rad/H/NonDeC
!CH3CH[OH]CHCH3+H2O2=sBuOH+HO2 2.9734435e+03     2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
O/H/NonDeO
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HO2+CH3CH[OH]CHCH3=H2O2+sC4H8O 7.2300000e+13     0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Csrad
C4H7-24+CH3CH[OH]CHCH3=C4H8-1+sC4H8O 6.3300000e+14     -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
CH3CH[OH]CHCH3+CH3CH[OH]CHCH3=sBuOH+sC4H8O 6.3300000e+14     -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
sC4H8O+HO2=CH3C[OH]CHcH2+H2O2 8.0670536e+08      0.95000     5448.25000
       !H_Abstraction estimate: (Average:)  C/H/ODMustO     O_rad/NonDeO
sC4H8O+C4H7-24=CH3C[OH]CHcH2+C4H8-1 1.6208066e+09      1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C/H/ODMustO
C_rad/H/OneDeC
sC4H8O+CH3CH[OH]CHCH3=CH3C[OH]CHcH2+sBuOH 1.6208066e+09      1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C/H/ODMustO
C_rad/H/NonDeC
C4H7-24+CH3C[OH]CHcH2=C4H6-13+sC4H8O 8.5800000e+15     -1.10000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/ODMustO
CH3CH[OH]CHCH3+CH3C[OH]CHcH2=sC4H8O+sC4H8O 8.5800000e+15     -1.10000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/ODMustO
HO2+CH3C[OH]CHcH2=H2O2+C4H6O(717) 1.2100000e+13        0.00000
0.00000      !Disproportionation exact:   O_rad/NonDeO     O_Csrad
C4H7-24+CH3C[OH]CHcH2=C4H8-1+C4H6O(717) 2.3500000e+12        0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
O_Csrad
OH+CH3C[OH]CHcH2=H2O+C4H6O(717) 2.4100000e+13    0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
CH3CH[OH]CHCH3+CH3C[OH]CHcH2=sBuOH+C4H6O(717) 2.3500000e+12
0.00000      0.00000     !Disproportionation exact:   C_rad/H/NonDeC
O_Csrad
CH3C[OH]CHcH2+CH3C[OH]CHcH2=sC4H8O+C4H6O(717) 3.4700000e+14        -
0.75000      0.00000     !Disproportionation estimate: (Average:)
C_rad/ODMustO     O_Csrad
!O2+CH3C[OH]CHcH2=HO2+C4H6O(717) 2.2800000e+13   0.00000     0.00000
!Disproportionation_O2d exact:   O2d     O_Csrad
O2+CH3C[OH]CHcH2=HO2+C4H6O(717)     4.6826e+11 0.3321 -1.0635e+03 !from
rate calculated by Zador et al for CH3CHOH+O2=HO2+CH3CHO (consistent
with RMG) edited by MRH 05.12.11
HO2+CH3CH[OH]CHCH3=H2O2+MEKenol 1.2100000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
C4H7-24+CH3CH[OH]CHCH3=C4H8-1+MEKenol 2.5600000e+13    -0.35000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H/NdNd_Csrad
CH3CH[OH]CHCH3+CH3CH[OH]CHCH3=sBuOH+MEKenol 2.5600000e+13    -0.35000
0.00000      !Disproportionation exact:   C/H/NdNd_Csrad
C_rad/H/NonDeC
CH3CH[OH]CHCH3+MEKenol=sBuOH+CH3C[OH]CHcH2 8.6100000e+11     0.00000
12300.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
C4H8-1+CH3C[OH]CHcH2=C4H7-24+MEKenol 3.0397882e+06     1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
C_rad/H2/Cd
H2O2+CH3C[OH]CHcH2=HO2+MEKenol 2.9734435e+03     2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     C_rad/H2/Cd
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CH3C[OH]CHcH2+CH3CH[OH]CHCH3=sC4H8O+MEKenol 1.0800000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/ODMustO
C/H/NdNd_Csrad
CH3C[OH]CHcH2+CH3C[OH]CHcH2=MEKenol+C4H6O(717) 1.8100000e+13
0.00000      0.00000     !Disproportionation exact:   O_Csrad
C_rad/H2/Cd
CH3C[OH]CHcH2+C4H7-24=MEKenol+C4H6-13 6.8700000e+13    -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
CH3C[OH]CHcH2+CH3CH[OH]CHCH3=MEKenol+MEKenol 7.8300000e+11   0.00000
-130.00000   !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
CH3C[O]cHCH3+CH3CH[OH]CHCH3=C4H6O(717)+sBuOH 6.3300000e+14   -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
CH3C[O]cHCH3+C4H7-24=C4H6O(717)+C4H8-1 6.3300000e+14   -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
CH3C[O]cHCH3+HO2=C4H6O(717)+H2O2 7.2300000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     O_rad/NonDeO
CH3C[O]cHCH3+CH3C[OH]CHcH2=C4H6O(717)+sC4H8O 8.5800000e+15   -1.10000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/ODMustO
!CH3C[O]cHCH3+H2O2=MEKenol+HO2 3.4600000e+01     3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     O/H/NonDeO
CH3C[O]cHCH3+H2O2=MEKenol+HO2 6.99e-02 3.75 10.89e+03  !MHS 04/29/11
(CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
CH3C[O]cHCH3+C4H8-1=MEKenol+C4H7-24 3.1729268e+09      0.95000
5644.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H2/OneDeC
MEKenol+CH3CH[OH]CHCH3=CH3C[O]cHCH3+sBuOH 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/NonDeC
CH3C[O]cHCH3+sC4H8O=MEKenol+CH3C[OH]CHcH2 8.0670536e+08      0.95000
5448.25000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H/ODMustO
MEKenol+CH3C[OH]CHcH2=CH3C[O]cHCH3+MEKenol 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cd
CH3C[O]cHCH3+CH3C[OH]CHcH2=C4H6O(717)+MEKenol 2.2900000e+13        -
0.35000      -130.00000        !Disproportionation exact:
Cmethyl_Csrad     C_rad/H2/Cd
HO2+CH3CH[OH]CH2CH2=O2+sBuOH 3.0000000e+11       0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
!CH3CH[OH]CH2CH2+H2O2=sBuOH+HO2 2.9734435e+03    2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cs     O/H/NonDeO
CH3CH[OH]CH2CH2+CH3CH[OH]CHCH3=sC4H8O+sBuOH  5.1300000e+13   -0.35000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
C/H2/Nd_Csrad
DUP
CH3CH[OH]CH2CH2+CH3CH[OH]CHCH3=sC4H8O+sBuOH  2.3000000e+13   -0.35000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
DUP
CH3CH[OH]CH2CH2+CH3CH[OH]CH2CH2=sC4H8O+sBuOH 2.9000000e+12   0.00000
0.00000      !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cs
CH3CH[OH]CH2CH2+C4H7-24=sC4H8O+C4H8-1 1.0260000e+14    -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H/OneDeC
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CH3CH[OH]CH2CH2+HO2=sC4H8O+H2O2 4.8200000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     O_rad/NonDeO
CH3CH[OH]CH2CH2+CH3C[OH]CHcH2=sC4H8O+sC4H8O 4.3200000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/ODMustO
CH3CH[OH]CH2CH2+sC4H8O=sBuOH+CH3C[OH]CHcH2 1.6208066e+09     1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H/ODMustO
CH3CH[OH]CH2CH2+MEKenol=sBuOH+CH3C[OH]CHcH2 1.6800000e+12    0.00000
12400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
CH3C[O]cHCH3+CH3CH[OH]CH2CH2=C4H6O(717)+sBuOH 6.9000000e+13        -
0.35000      0.00000     !Disproportionation exact:   Cmethyl_Csrad
C_rad/H2/Cs
CH3C[OH]CHcH2+CH3CH[OH]CH2CH2=C4H6O(717)+sBuOH 2.4100000e+12
0.00000      0.00000     !Disproportionation exact:   O_Csrad
C_rad/H2/Cs
CH3CH[OH]CHCH3+CH3CH[OH]CH2CH2=MEKenol+sBuOH 8.4300000e+11   0.00000
0.00000      !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cs
CH3CH[OH]CH2CH2+CH3C[OH]CHcH2=sC4H8O+MEKenol 2.9000000e+12   0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
CH3CH[OH]CH2CH2+MEKenol=sBuOH+CH3C[O]cHCH3 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/OneDe
HO2+sSPC(1013)=H2O2+sSPC(1072) 1.2100000e+13     0.00000     0.00000
!Disproportionation exact:   O_Csrad     O_rad/NonDeO
C4H7-24+sSPC(1013)=C4H8-1+sSPC(1072) 2.3500000e+12     0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
O_Csrad
OH+sSPC(1013)=H2O+sSPC(1072) 2.4100000e+13       0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
CH3CH[OH]CHCH3+sSPC(1013)=sBuOH+sSPC(1072) 2.3500000e+12     0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H/NonDeC
CH3C[OH]CHcH2+sSPC(1013)=sC4H8O+sSPC(1072) 3.4700000e+14     -0.75000
0.00000      !Disproportionation estimate: (Average:)  C_rad/ODMustO
O_Csrad
CH3C[OH]CHcH2+sSPC(1013)=MEKenol+sSPC(1072) 1.8100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
CH3C[O]cHCH3+sSPC(1013)=MEKenol+sSPC(1072) 1.7076592e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/OneDe
O_Csrad
CH3CH[OH]CH2CH2+sSPC(1013)=sBuOH+sSPC(1072) 2.4100000e+12    0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cs
!O2+sSPC(1013)=HO2+sSPC(1072) 2.2800000e+13      0.00000     0.00000
!Disproportionation_O2d exact:   O2d     O_Csrad
O2+sSPC(1013)=HO2+sSPC(1072)  4.6826e+11 0.3321 -1.0635e+03 !from rate
calculated by Zador et al for CH3CHOH+O2=HO2+CH3CHO (consistent with
RMG) edited by MRH 05.12.11
CH3CH[OH]CHCH3+sSPC(1735)=sBuOH+sSPC(1697) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
O/H/NonDeO
CH3CH[OH]CH2CH2+sSPC(1735)=sBuOH+sSPC(1697) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
OH+sSPC(1735)=H2O+sSPC(1697) 1.7300000e+01       3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_pri_rad     O/H/NonDeO
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C4H8-1+sSPC(1697)=C4H7-24+sSPC(1735) 3.1729268e+09     0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
O_rad/NonDeO
H2O2+sSPC(1697)=HO2+sSPC(1735) 3.4600000e+01     3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     O_rad/NonDeO
sC4H8O+sSPC(1697)=CH3C[OH]CHcH2+sSPC(1735) 8.0670536e+08     0.95000
5448.25000   !H_Abstraction estimate: (Average:)  C/H/ODMustO
O_rad/NonDeO
CH3C[OH]CHcH2+sSPC(1735)=MEKenol+sSPC(1697) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
!CH3C[O]cHCH3+sSPC(1735)=MEKenol+sSPC(1697) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH3C[O]cHCH3+sSPC(1735)=MEKenol+sSPC(1697)      6.99e-02 3.75 10.89e+03
!MHS 04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
sSPC(1697)+HO2=sSPC(1735)+O2 1.7500000e+10       0.00000     -3275.00000
       !Disproportionation estimate: (Average:)  O_rad/NonDeO     O_Orad
sSPC(1697)+C4H7-24=sSPC(1735)+C4H6-13 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(1697)+CH3CH[OH]CHCH3=sSPC(1735)+sC4H8O 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(1697)+CH3CH[OH]CHCH3=sSPC(1735)+MEKenol 1.2100000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
sSPC(1697)+CH3C[OH]CHcH2=sSPC(1735)+C4H6O(717) 1.2100000e+13
0.00000      0.00000     !Disproportionation exact:   O_Csrad
O_rad/NonDeO
sSPC(1697)+CH3C[O]cHCH3=sSPC(1735)+C4H6O(717) 7.2300000e+13
0.00000      0.00000     !Disproportionation estimate: (Average:)
O_rad/NonDeO     Cmethyl_Csrad
sSPC(1697)+CH3CH[OH]CH2CH2=sSPC(1735)+sC4H8O 4.8200000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
sSPC(1697)+sSPC(1013)=sSPC(1735)+sSPC(1072) 1.2100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     O_rad/NonDeO
CH3O+CH3CH[OH]CHCH3=CH2O+sBuOH 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad
C_rad/H/NonDeC
CH3O+CH3CH[OH]CH2CH2=CH2O+sBuOH 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_rad/H2/Cs
CH3O+C4H7-24=CH2O+C4H8-1 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad
C_rad/H/OneDeC
CH3O+HO2=CH2O+H2O2 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/NonDeO
CH3O+CH3C[OH]CHcH2=CH2O+sC4H8O 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_rad/ODMustO
CH3O+CH3C[OH]CHcH2=CH2O+MEKenol 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_rad/H2/Cd
CH3O+CH3C[O]cHCH3=CH2O+MEKenol 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/OneDe
CH3O+sSPC(1697)=CH2O+sSPC(1735) 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/NonDeO
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HO2+CH2=O2+CH3 1.0458681e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     CH2_triplet
C4H7-24+CH2=C4H6-13+CH3 9.0300000e+13      0.00000     0.00000
!Disproportionation exact:   CH2_triplet     Cmethyl_Csrad
CH3CH[OH]CH2CH2+CH2=sC4H8O+CH3 3.6200000e+12     0.00000     0.00000
!Disproportionation exact:   CH2_triplet     C/H2/Nd_Csrad
CH3CH[OH]CHCH3+CH2=sC4H8O+CH3 9.0300000e+13      0.00000     0.00000
!Disproportionation exact:   CH2_triplet     Cmethyl_Csrad
CH3C[O]cHCH3+CH2=C4H6O(717)+CH3 9.0300000e+13    0.00000     0.00000
!Disproportionation exact:   CH2_triplet     Cmethyl_Csrad
CH3C[OH]CHcH2+CH2=C4H6O(717)+CH3 1.2100000e+12   0.00000     0.00000
!Disproportionation exact:   CH2_triplet     O_Csrad
CH3CH[OH]CHCH3+CH2=MEKenol+CH3 7.7460197e+12     -0.06091    -63.81982
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad     CH2_triplet
sSPC(1013)+CH2=sSPC(1072)+CH3 1.2100000e+12      0.00000     0.00000
!Disproportionation exact:   CH2_triplet     O_Csrad
CH3O+CH2=CH2O+CH3 9.0300000e+13      0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Orad     CH2_triplet
sBuOH+CH2=CH3CH[OH]CHCH3+CH3 1.5100000e+00       3.46000     7470.00000
       !H_Abstraction exact:   C/H2/NonDeC     CH2_triplet
sBuOH+CH2=CH3CH[OH]CH2CH2+CH3 3.6429120e+05      2.34400     3744.60000
       !H_Abstraction estimate: (Average:)  C/H3/Cs     CH2_triplet
C4H8-1+CH2=C4H7-24+CH3 1.5100000e+00       3.46000     7470.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     CH2_triplet
H2O2+CH2=HO2+CH3 2.8800000e+01       3.10000     6940.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     CH2_triplet
sC4H8O+CH2=CH3C[OH]CHcH2+CH3 1.0900000e+12       0.00000     4910.00000
       !H_Abstraction estimate: (Average:)  C/H/ODMustO     CH2_triplet
MEKenol+CH2=CH3C[O]cHCH3+CH3 1.4400000e+01       3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     CH2_triplet
sSPC(1735)+CH2=sSPC(1697)+CH3 1.4400000e+01      3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     CH2_triplet
CH3CH[OH]CH2CH2+O=sC4H8O+OH 3.6200000e+12        0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_atom_triplet
CH3CH[OH]CHCH3+O=sC4H8O+OH 9.0300000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_atom_triplet
CH3C[O]cHCH3+O=C4H6O(717)+OH 9.0300000e+13       0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_atom_triplet
CH3CH[OH]CHCH3+O=MEKenol+OH 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_atom_triplet
sBuOH+O=CH3CH[OH]CHCH3+OH 4.7800000e+04    2.71000     2110.00000
!H_Abstraction exact:   C/H2/NonDeC     O_atom_triplet
sBuOH+O=CH3CH[OH]CH2CH2+OH 2.5650000e+04   3.05000     3123.00000
!H_Abstraction exact:   C/H3/Cs     O_atom_triplet
C4H8-1+O=C4H7-24+OH 4.7800000e+04    2.71000     2110.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     O_atom_triplet
sC4H8O+O=CH3C[OH]CHcH2+OH 1.5700000e+05    2.50000     1110.00000
!H_Abstraction estimate: (Average:)  C/H/ODMustO     O_atom_triplet
MEKenol+O=CH3C[OH]CHcH2+OH 2.5650000e+04   3.05000     3123.00000
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_atom_triplet
sSPC(1735)+O=sSPC(1697)+OH 1.0000000e+13   0.00000     4690.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     O_atom_triplet
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HCO+C4H8-1=CH2O+C4H7-24 7.5657121e+06      1.95000     16625.00000
!H_Abstraction estimate: (Average:)  CO_pri_rad     C/H2/OneDeC
CH2O+CH3CH[OH]CHCH3=HCO+sBuOH 1.0800000e+11      0.00000     6960.00000
       !H_Abstraction exact:   C_rad/H/NonDeC     CO_pri
HCO+sC4H8O=CH2O+CH3C[OH]CHcH2 3.4300000e+04      2.50000     13510.00000
       !H_Abstraction estimate: (Average:)  CO_pri_rad     C/H/ODMustO
CH2O+CH3C[OH]CHcH2=HCO+MEKenol 5.5000000e+03     2.81000     5860.00000
       !H_Abstraction estimate: (Average:)  CO_pri     C_rad/H2/Cd
CH2O+CH3C[O]cHCH3=HCO+MEKenol 6.4825921e+07      1.25000     6595.00000
       !H_Abstraction estimate: (Average:)  CO_pri     O_rad/OneDe
CH2O+CH3CH[OH]CH2CH2=HCO+sBuOH 5.5000000e+03     2.81000     5860.00000
       !H_Abstraction exact:   C_rad/H2/Cs     CO_pri
C4H7-24+HCO=C4H6-13+CH2O 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_pri_rad
CH3CH[OH]CH2CH2+HCO=sC4H8O+CH2O 1.1401172e+13    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     CO_pri_rad
CH3CH[OH]CHCH3+HCO=sC4H8O+CH2O 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_pri_rad
CH3C[O]cHCH3+HCO=C4H6O(717)+CH2O 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_pri_rad
CH3C[OH]CHcH2+HCO=C4H6O(717)+CH2O 1.8100000e+14        0.00000
0.00000      !Disproportionation exact:   CO_pri_rad     O_Csrad
CH3CH[OH]CHCH3+HCO=MEKenol+CH2O 3.5218932e+12    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad     CO_pri_rad
sSPC(1013)+HCO=sSPC(1072)+CH2O 1.8100000e+14     0.00000     0.00000
!Disproportionation exact:   CO_pri_rad     O_Csrad
CH3O+HCO=CH2O+CH2O 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     CO_pri_rad
CH2O+sSPC(1697)=HCO+sSPC(1735) 4.1200000e+04     2.50000     10210.00000
       !H_Abstraction exact:   O_rad/NonDeO     CO_pri
CH2O+CH2=HCO+CH3 6.0400000e+09       0.00000     0.00000
!H_Abstraction exact:   CO_pri     CH2_triplet
CH3CH[OH]CHCH3+sSPC(3121)=sBuOH+sSPC(3071) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
O/H/NonDeO
CH3CH[OH]CH2CH2+sSPC(3121)=sBuOH+sSPC(3071) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
OH+sSPC(3121)=H2O+sSPC(3071) 1.7300000e+01       3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_pri_rad     O/H/NonDeO
C4H8-1+sSPC(3071)=C4H7-24+sSPC(3121) 3.1729268e+09     0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
O_rad/NonDeO
H2O2+sSPC(3071)=HO2+sSPC(3121) 3.4600000e+01     3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     O_rad/NonDeO
sC4H8O+sSPC(3071)=CH3C[OH]CHcH2+sSPC(3121) 8.0670536e+08     0.95000
5448.25000   !H_Abstraction estimate: (Average:)  C/H/ODMustO
O_rad/NonDeO
MEKenol+sSPC(3071)=CH3C[OH]CHcH2+sSPC(3121) 3.4482017e+07    1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeO
MEKenol+sSPC(3071)=CH3C[O]cHCH3+sSPC(3121) 1.7300000e+01     3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeO
CH2O+sSPC(3071)=HCO+sSPC(3121) 4.1200000e+04     2.50000     10210.00000
       !H_Abstraction exact:   CO_pri     O_rad/NonDeO
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sSPC(1735)+sSPC(3071)=sSPC(1697)+sSPC(3121) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/NonDeO
O_rad/NonDeO
sSPC(3071)+HO2=sSPC(3121)+O2 1.7500000e+10       0.00000     -3275.00000
       !Disproportionation estimate: (Average:)  O_rad/NonDeO     O_Orad
sSPC(3071)+C4H7-24=sSPC(3121)+C4H6-13 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(3071)+CH3CH[OH]CHCH3=sSPC(3121)+sC4H8O 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(3071)+CH3CH[OH]CHCH3=sSPC(3121)+MEKenol 1.2100000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
sSPC(3071)+CH3C[OH]CHcH2=sSPC(3121)+C4H6O(717) 1.2100000e+13
0.00000      0.00000     !Disproportionation exact:   O_Csrad
O_rad/NonDeO
sSPC(3071)+CH3C[O]cHCH3=sSPC(3121)+C4H6O(717) 7.2300000e+13
0.00000      0.00000     !Disproportionation estimate: (Average:)
O_rad/NonDeO     Cmethyl_Csrad
sSPC(3071)+CH3CH[OH]CH2CH2=sSPC(3121)+sC4H8O 4.8200000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
sSPC(3071)+sSPC(1013)=sSPC(3121)+sSPC(1072) 1.2100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     O_rad/NonDeO
sSPC(3071)+CH3O=sSPC(3121)+CH2O 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Orad
sSPC(3121)+CH2=sSPC(3071)+CH3 1.4400000e+01      3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     CH2_triplet
sSPC(2810)+OH=CO2+H2O 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Orad     O_pri_rad
sSPC(2810)+HO2=CO2+H2O2 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Orad     O_rad/NonDeO
sSPC(2810)+CH3C[O]cHCH3=CO2+MEKenol 7.7460197e+12      -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Orad
O_rad/OneDe
sSPC(2810)+HCO=CO2+CH2O 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Orad     CO_pri_rad
sSPC(2810)+CH2=CO2+CH3 7.7460197e+12       -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Orad     CH2_triplet
sSPC(2810)+sSPC(1697)=CO2+sSPC(1735) 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Orad
O_rad/NonDeO
O2+sSPC(2810)=HO2+CO2 6.5566084e+11        0.00000     2710.00000
!Disproportionation_O2d estimate: (Average:)  O2d     COpri_Orad
sSPC(2810)+sSPC(3071)=CO2+sSPC(3121) 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Orad
O_rad/NonDeO
CH3CH[OH]CHCH3+sSPC(1474)=sBuOH+sSPC(1356) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
O/H/NonDeO
CH3CH[OH]CH2CH2+sSPC(1474)=sBuOH+sSPC(1356) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
OH+sSPC(1474)=H2O+sSPC(1356) 1.7300000e+01       3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_pri_rad     O/H/NonDeO
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C4H8-1+sSPC(1356)=C4H7-24+sSPC(1474) 3.1729268e+09     0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeC
O_rad/NonDeO
H2O2+sSPC(1356)=HO2+sSPC(1474) 3.4600000e+01     3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     O_rad/NonDeO
sC4H8O+sSPC(1356)=CH3C[OH]CHcH2+sSPC(1474) 8.0670536e+08     0.95000
5448.25000   !H_Abstraction estimate: (Average:)  C/H/ODMustO
O_rad/NonDeO
CH3C[OH]CHcH2+sSPC(1474)=MEKenol+sSPC(1356) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
!CH3C[O]cHCH3+sSPC(1474)=MEKenol+sSPC(1356) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH3C[O]cHCH3+sSPC(1474)=MEKenol+sSPC(1356)      6.99e-02 3.75 10.89e+03
!MHS 04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
CH2O+sSPC(1356)=HCO+sSPC(1474) 4.1200000e+04     2.50000     10210.00000
       !H_Abstraction exact:   CO_pri     O_rad/NonDeO
sSPC(1356)+HO2=sSPC(1474)+O2 1.7500000e+10       0.00000     -3275.00000
       !Disproportionation estimate: (Average:)  O_rad/NonDeO     O_Orad
sSPC(1356)+C4H7-24=sSPC(1474)+C4H6-13 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(1356)+CH3CH[OH]CHCH3=sSPC(1474)+sC4H8O 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cmethyl_Csrad
sSPC(1356)+CH3CH[OH]CHCH3=sSPC(1474)+MEKenol 1.2100000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
sSPC(1356)+CH3C[OH]CHcH2=sSPC(1474)+C4H6O(717) 1.2100000e+13
0.00000      0.00000     !Disproportionation exact:   O_Csrad
O_rad/NonDeO
sSPC(1356)+CH3C[O]cHCH3=sSPC(1474)+C4H6O(717) 7.2300000e+13
0.00000      0.00000     !Disproportionation estimate: (Average:)
O_rad/NonDeO     Cmethyl_Csrad
sSPC(1356)+CH3CH[OH]CH2CH2=sSPC(1474)+sC4H8O 4.8200000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H2/Nd_Csrad
sSPC(1356)+sSPC(1013)=sSPC(1474)+sSPC(1072) 1.2100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     O_rad/NonDeO
sSPC(1735)+sSPC(1356)=sSPC(1697)+sSPC(1474) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/NonDeO
O_rad/NonDeO
sSPC(1356)+CH3O=sSPC(1474)+CH2O 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Orad
sSPC(3071)+sSPC(1474)=sSPC(3121)+sSPC(1356) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/NonDeO
sSPC(1356)+sSPC(2810)=sSPC(1474)+CO2 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Orad
sSPC(1474)+CH2=sSPC(1356)+CH3 1.4400000e+01      3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     CH2_triplet
sSPC(1474)+O=sSPC(1356)+OH 1.0000000e+13   0.00000     4690.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     O_atom_triplet
CH3CO+HO2=CH2CO+H2O2 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     O_rad/NonDeO
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CH3CO+O=CH2CO+OH 9.0300000e+13       0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_COrad
O_atom_triplet
CH3CO+CH3C[OH]CHcH2=CH2CO+sC4H8O 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad
C_rad/ODMustO
CH3CO+CH3C[OH]CHcH2=CH2CO+MEKenol 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
C_rad/H2/Cd
CH3CO+HCO=CH2CO+CH2O 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     CO_pri_rad
CH3CO+CH2=CH2CO+CH3 9.0300000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_COrad     CH2_triplet
CH3CO+sSPC(1697)=CH2CO+sSPC(1735) 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
O_rad/NonDeO
CH3CO+sSPC(3071)=CH2CO+sSPC(3121) 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
O_rad/NonDeO
CH3CO+sSPC(1356)=CH2CO+sSPC(1474) 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
O_rad/NonDeO

sBuOH+O=CH2CH[OH]C2H5+OH      25650.0     3.05  3.123e+03
      !H_Abstraction exact:   C/H3/Cs     O_atom_triplet
sBuOH+O=CH3C[OH]C2H5+OH       157000.0    2.5   1.11e+03
      !H_Abstraction estimate: (Average:) C/H/NDMustO     O_atom_triplet
sBuOH+O=CH3CH[O]C2H5+OH       1.0E13      0.0   4.69e+03
      !H_Abstraction exact:   O/H/NonDeC     O_atom_triplet
!CH2CH[OH]C2H5+H2O2=sBuOH+HO2       2973.44     2.386 9.690e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     O/H/NonDeO
!CH3C[OH]C2H5+H2O2=sBuOH+HO2        2973.44     2.386 9.690e+03
      !H_Abstraction estimate: (Average:) C_rad/NDMustO     O/H/NonDeO
CH3CH[O]C2H5+H2O2=sBuOH+HO2         34.6        3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeO
HO2+CH2CH[OH]C2H5=O2+sBuOH    3.00E11     0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
HO2+CH3C[OH]C2H5=O2+sBuOH     3.00E11     0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/NDMustO
HO2+CH3CH[O]C2H5=O2+sBuOH     1.75E10     0.0   -3.275e+03
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/NonDeC

!C4H6O(105)(+m)=C3H3O-enone+CH3(+m) 1.0E0 0.0 0.0
!TCHEB / 300.0 2100.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 4   4 /
!CHEB / -1.6740000e+01 1.7094000e-01 -1.8065000e-01 -5.1938000e-02 /
!CHEB / 2.1229000e+01 8.3321000e-01 3.5543000e-02 3.8982000e-02 /
!CHEB / -5.7048000e-01 3.6773000e-01 -2.3733000e-02 -8.0498000e-03 /
!CHEB / -3.3817000e-01 1.2945000e-01 1.1044000e-02 -1.1964000e-02 /


!tSPC(346)+CH3(+m)=C3H3O-enone+CH3(+m)    1.0E0 0.0 0.0
!TCHEB / 300.0 2100.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 4   4 /
!CHEB / 4.2460000e+00 -8.9074000e-01 6.0522000e-02 -6.0444000e-03 /
!CHEB / 4.9952000e+00 6.5832000e-01 -1.4786000e-01 2.8178000e-02 /
!CHEB / 1.1349000e-01 2.9241000e-01 5.5526000e-03 -4.4995000e-02 /
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!CHEB / -1.8479000e-01 -2.8260000e-03 7.6180000e-02 3.8859000e-03 /


HO2+iC4H7=O2+iC4H8 3.0000000e+11     0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cd
HO2+HOC[CH2][CH3]2=O2+tBuOH 3.0000000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
iC4H7+tSPC(346)=iC4H8+H2CCCO 7.7460197e+12       -0.06091    -63.81982
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     COpri_Cdrad
OH+tSPC(346)=H2O+H2CCCO 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  O_pri_rad     COpri_Cdrad
HOC[CH2][CH3]2+tSPC(346)=tBuOH+H2CCCO 7.7460197e+12    -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H2/Cs
COpri_Cdrad
CH3+tSPC(346)=CH4+H2CCCO 7.7460197e+12     -0.06091    -63.81982
!Disproportionation estimate: (Average:)  C_methyl     COpri_Cdrad
C3H3O-enone+HOC[CH2][CH3]2=H2CCCO+tBuOH 9.6400000e+11        0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cs     Cdpri_Csrad
C3H3O-enone+iC4H7=H2CCCO+iC4H8 8.4300000e+10     0.00000     -260.00000
       !Disproportionation exact:   C_rad/H2/Cd     Cdpri_Csrad
C3H3O-enone+OH=H2CCCO+H2O 6.0300000e+12    0.00000     0.00000
!Disproportionation exact:   O_pri_rad     Cdpri_Csrad
C3H3O-enone+CH3=H2CCCO+CH4 3.0100000e+12   -0.32000    -130.00000
!Disproportionation exact:   C_methyl     Cdpri_Csrad
HOC[CH2][CH3]2+tSPC(1416)=tBuOH+tSPC(1286) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
iC4H8+tSPC(1286)=iC4H7+tSPC(1416) 6.8964034e+07        1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeO
OH+tSPC(1416)=H2O+tSPC(1286) 1.7300000e+01       3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_pri_rad     O/H/NonDeO
CH3+tSPC(1416)=CH4+tSPC(1286) 1.4867217e+03      2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_methyl     O/H/NonDeO
tSPC(1286)+HO2=tSPC(1416)+O2 1.7500000e+10       0.00000     -3275.00000
       !Disproportionation estimate: (Average:)  O_rad/NonDeO     O_Orad
tSPC(1286)+tSPC(346)=tSPC(1416)+H2CCCO 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Cdrad
tSPC(1286)+C3H3O-enone=tSPC(1416)+H2CCCO 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_COrad
tSPC(346)+O=H2CCCO+OH 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Cdrad     O_atom_triplet
!tBuOH+O=HOC[CH2][CH3]2+OH 3.50000e+04     3.05000     3123.00000
!H_Abstraction exact:   C/H3/Cs     O_atom_triplet
tBuOH+O=HOC[CH2][CH3]2+OH     4.28e+05    2.5   3.64e+03
      !iC4H10+O=OH+iC4H9 (Tsang)
iC4H8+O=iC4H7+OH 2.5700000e+04       3.05000     3123.00000
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_atom_triplet
HOC[CH2][CH3]2+C2H4O=tBuOH+CH2CHO 1.4867217e+03        2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/OneDe
iC4H8+CH2CHO=iC4H7+C2H4O 6.8964034e+07     1.75000     3789.37500
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_rad/OneDe
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tSPC(1286)+C2H4O=tSPC(1416)+CH2CHO 1.7300000e+01       3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/OneDe
CH2CHO+HO2=C2H4O+O2 1.7500000e+10    0.00000     -3275.00000
!Disproportionation estimate: (Average:)  O_rad/OneDe     O_Orad
CH2CHO+tSPC(346)=C2H4O+H2CCCO 7.7460197e+12      -0.06091    -63.81982
!Disproportionation estimate: (Average:)  O_rad/OneDe     COpri_Cdrad
CH2CHO+C3H3O-enone=C2H4O+H2CCCO 5.4132535e+12    -0.08875    -36.56250
!Disproportionation estimate: (Average:)  O_rad/OneDe     Cdpri_COrad
HO2+CH2C[O]CH3=O2+H2CCCH3[OH] 1.7500000e+10      0.00000     -3275.00000
       !Disproportionation estimate: (Average:)  O_Orad     O_rad/OneDe
C3H3O-enone+CH2C[O]CH3=H2CCCO+H2CCCH3[OH] 6.0300000e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  Cdpri_Csrad
O_rad/OneDe
tSPC(346)+CH2C[O]CH3=H2CCCO+H2CCCH3[OH] 7.7460197e+12        -0.06091
-63.81982    !Disproportionation estimate: (Average:)  COpri_Cdrad
O_rad/OneDe
H2CCCH3[OH]+tSPC(1286)=CH2C[O]CH3+tSPC(1416) 1.7300000e+01   3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeO
iC4H7+CH2CHO=iC4H8+CH2CO 5.4132535e+12     -0.08875    -36.56250
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cdpri_Orad
HOC[CH2][CH3]2+CH2CHO=tBuOH+CH2CO 5.4132535e+12        -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  C_rad/H2/Cs
Cdpri_Orad
tSPC(1286)+CH2CHO=tSPC(1416)+CH2CO 5.4132535e+12       -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Orad
HOC[CH2][CH3]2+sSPC(1735)=tBuOH+sSPC(1697) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
iC4H7+sSPC(1735)=iC4H8+sSPC(1697) 1.4867217e+03        2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
!CH2C[O]CH3+sSPC(1735)=H2CCCH3[OH]+sSPC(1697) 1.7300000e+01
3.40000      -1140.00000       !H_Abstraction estimate: (Average:)
O_rad/OneDe     O/H/NonDeO
CH2C[O]CH3+sSPC(1735)=H2CCCH3[OH]+sSPC(1697)    6.99e-02 3.75 10.89e+03
!MHS 04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
CH3+sSPC(1735)=CH4+sSPC(1697) 1.4867217e+03      2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_methyl     O/H/NonDeO
sSPC(1697)+tSPC(346)=sSPC(1735)+H2CCCO 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Cdrad
sSPC(1697)+C3H3O-enone=sSPC(1735)+H2CCCO 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_COrad
tSPC(1286)+sSPC(1735)=tSPC(1416)+sSPC(1697) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/NonDeO
sSPC(1697)+CH2CHO=sSPC(1735)+CH2CO 5.4132535e+12       -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Orad
CH2CHO+sSPC(1735)=C2H4O+sSPC(1697) 6.99e-02 3.75 10.89e+03  !MHS
04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
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!CH2CHO+sSPC(1735)=C2H4O+sSPC(1697) 1.7300000e+01      3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH3O+HOC[CH2][CH3]2=CH2O+tBuOH 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_rad/H2/Cs
CH3O+iC4H7=CH2O+iC4H8 7.0652342e+13        -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_rad/H2/Cd
CH3O+CH2C[O]CH3=CH2O+H2CCCH3[OH] 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/OneDe
CH3O+CH3=CH2O+CH4 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     C_methyl
CH3O+tSPC(1286)=CH2O+tSPC(1416) 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/NonDeO
CH3O+CH2CHO=CH2O+C2H4O 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     O_rad/OneDe
!HOC[CH2][CH3]2+H2O2=tBuOH+HO2 2.9734435e+03     2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cs     O/H/NonDeO
iC4H7+H2O2=iC4H8+HO2 2.9734435e+03   2.38600     9690.00000
!H_Abstraction estimate: (Average:)  C_rad/H2/Cd     O/H/NonDeO
!CH2C[O]CH3+H2O2=H2CCCH3[OH]+HO2 3.4600000e+01   3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     O/H/NonDeO
!H2CCCH3[OH]+HO2=CH2C[O]CH3+H2O2    17.3  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_rad/NonDeO
      deltaHrxn(T=298K) = -2.3296393870731613 kcal/mol
H2CCCH3[OH]+HO2=CH2C[O]CH3+H2O2           9.63e+03    2.6   13.91e+03
      ! C3H6+HO2=H2O2+aC3H5 (Tsang)
HO2+tSPC(346)=H2O2+H2CCCO 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  O_rad/NonDeO     COpri_Cdrad
HO2+C3H3O-enone=H2O2+H2CCCO 5.4132535e+12        -0.08875    -36.56250
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cdpri_COrad
tSPC(1286)+H2O2=tSPC(1416)+HO2 3.4600000e+01     3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O_rad/NonDeO     O/H/NonDeO
!CH2CHO+H2O2=C2H4O+HO2 3.4600000e+01       3.40000     -1140.00000
!H_Abstraction estimate: (Average:)  O_rad/OneDe     O/H/NonDeO
HOC[CH2][CH3]2+sSPC(1474)=tBuOH+sSPC(1356) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
iC4H7+sSPC(1474)=iC4H8+sSPC(1356) 1.4867217e+03        2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
!CH2C[O]CH3+sSPC(1474)=H2CCCH3[OH]+sSPC(1356) 1.7300000e+01
3.40000      -1140.00000       !H_Abstraction estimate: (Average:)
O_rad/OneDe     O/H/NonDeO
CH2C[O]CH3+sSPC(1474)=H2CCCH3[OH]+sSPC(1356)    6.99e-02 3.75 10.89e+03
!MHS 04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
CH3+sSPC(1474)=CH4+sSPC(1356) 1.4867217e+03      2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_methyl     O/H/NonDeO
tSPC(1286)+sSPC(1474)=tSPC(1416)+sSPC(1356) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/NonDeO
!CH2CHO+sSPC(1474)=C2H4O+sSPC(1356) 1.7300000e+01      3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH2CHO+sSPC(1474)=C2H4O+sSPC(1356)  6.99e-02 3.75 10.89e+03  !MHS
04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
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sSPC(1356)+tSPC(346)=sSPC(1474)+H2CCCO 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Cdrad
sSPC(1356)+C3H3O-enone=sSPC(1474)+H2CCCO 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_COrad
sSPC(1356)+CH2CHO=sSPC(1474)+CH2CO 5.4132535e+12       -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Orad
HOC[CH2][CH3]2+sSPC(1474)=tBuOH+tSPC(3683) 9.4074532e+06     1.75273
12532.12121        !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H3/CO
iC4H8+tSPC(3683)=iC4H7+sSPC(1474) 1.7434638e+13        0.00000
17333.33333        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H2/CO
OH+sSPC(1474)=H2O+tSPC(3683) 1.5510000e+06       2.20000     1000.00000
       !H_Abstraction exact:   C/H3/CO     O_pri_rad
H2CCCH3[OH]+tSPC(3683)=CH2C[O]CH3+sSPC(1474) 1.4867217e+03   2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/CO
CH3+sSPC(1474)=CH4+tSPC(3683) 9.4074532e+06      1.75273     12532.12121
       !H_Abstraction estimate: (Average:)  C_methyl     C/H3/CO
tSPC(1416)+tSPC(3683)=tSPC(1286)+sSPC(1474) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/NonDeO
C_rad/H2/CO
C2H4O+tSPC(3683)=CH2CHO+sSPC(1474) 1.4867217e+03       2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/CO
tSPC(3683)+HO2=sSPC(1474)+O2 3.0000000e+11       0.00000     0.00000
!Disproportionation estimate: (Average:)  C_rad/H2/CO     O_Orad
tSPC(3683)+tSPC(346)=sSPC(1474)+H2CCCO 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H2/CO
COpri_Cdrad
tSPC(3683)+C3H3O-enone=sSPC(1474)+H2CCCO 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  C_rad/H2/CO
Cdpri_COrad
tSPC(3683)+CH2CHO=sSPC(1474)+CH2CO 5.4132535e+12       -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  C_rad/H2/CO
Cdpri_Orad
sSPC(1735)+tSPC(3683)=sSPC(1697)+sSPC(1474) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/NonDeO
C_rad/H2/CO
tSPC(3683)+CH3O=sSPC(1474)+CH2O 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/CO     Cmethyl_Orad
H2O2+tSPC(3683)=HO2+sSPC(1474) 2.9734435e+03     2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     C_rad/H2/CO
sSPC(1474)+O=tSPC(3683)+OH 2.5650000e+04   3.05000     3123.00000
!H_Abstraction estimate: (Average:)  C/H3/CO     O_atom_triplet
tSPC(3683)+sSPC(1474)=sSPC(1474)+sSPC(1356) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
O/H/NonDeO
CH3CO+HOC[CH2][CH3]2=CH2CO+tBuOH 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     C_rad/H2/Cs
CH3CO+iC4H7=CH2CO+iC4H8 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     C_rad/H2/Cd
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CH3CO+tSPC(1286)=CH2CO+tSPC(1416) 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
O_rad/NonDeO
CH3CO+tSPC(3683)=CH2CO+sSPC(1474) 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_COrad
C_rad/H2/CO
!CH2O+iC4H7=HCO+iC4H8 5.5000000e+03        2.81000     5860.00000
!H_Abstraction estimate: (Average:)  CO_pri     C_rad/H2/Cd
CH2O+HOC[CH2][CH3]2=HCO+tBuOH 5.5000000e+03      2.81000     5860.00000
       !H_Abstraction exact:   C_rad/H2/Cs     CO_pri
C3H3O-enone+HCO=H2CCCO+CH2O 5.4132535e+12        -0.08875    -36.56250
!Disproportionation estimate: (Average:)  Cdpri_Csrad     CO_pri_rad
tSPC(346)+HCO=H2CCCO+CH2O 7.7460197e+12    -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Cdrad     CO_pri_rad
CH2O+tSPC(1286)=HCO+tSPC(1416) 4.1200000e+04     2.50000     10210.00000
       !H_Abstraction exact:   O_rad/NonDeO     CO_pri
CH2O+CH2CHO=HCO+C2H4O 6.4825921e+07        1.25000     6595.00000
!H_Abstraction estimate: (Average:)  CO_pri     O_rad/OneDe
CH2O+CH2C[O]CH3=HCO+H2CCCH3[OH] 6.4825921e+07    1.25000     6595.00000
       !H_Abstraction estimate: (Average:)  CO_pri     O_rad/OneDe
CH2O+tSPC(3683)=HCO+sSPC(1474) 5.5000000e+03     2.81000     5860.00000
       !H_Abstraction estimate: (Average:)  CO_pri     C_rad/H2/CO
CH2CHO+HCO=CH2CO+CH2O 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Csrad     CO_pri_rad
HOC[CH2][CH3]2+sSPC(3121)=tBuOH+sSPC(3071) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
iC4H8+sSPC(3071)=iC4H7+sSPC(3121) 6.8964034e+07        1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeO
H2CCCH3[OH]+sSPC(3071)=CH2C[O]CH3+sSPC(3121) 1.7300000e+01   3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeO
CH3+sSPC(3121)=CH4+sSPC(3071) 1.4867217e+03      2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_methyl     O/H/NonDeO
tSPC(1416)+sSPC(3071)=tSPC(1286)+sSPC(3121) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/NonDeO
O_rad/NonDeO
C2H4O+sSPC(3071)=CH2CHO+sSPC(3121) 1.7300000e+01       3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeO
tSPC(3683)+sSPC(3121)=sSPC(1474)+sSPC(3071) 1.4867217e+03    2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
O/H/NonDeO
sSPC(3071)+tSPC(346)=sSPC(3121)+H2CCCO 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Cdrad
sSPC(3071)+C3H3O-enone=sSPC(3121)+H2CCCO 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_COrad
sSPC(3071)+CH2CHO=sSPC(3121)+CH2CO 5.4132535e+12       -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_Orad
sSPC(2810)+CH2C[O]CH3=CO2+H2CCCH3[OH] 7.7460197e+12    -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Orad
O_rad/OneDe
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sSPC(2810)+tSPC(1286)=CO2+tSPC(1416) 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Orad
O_rad/NonDeO
sSPC(2810)+CH2CHO=CO2+C2H4O 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  COpri_Orad     O_rad/OneDe
tSPC(1416)+H=tSPC(1286)+H2 1.0634848e+10   1.10500     8910.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     H_rad
sSPC(1735)+H=sSPC(1697)+H2 1.0634848e+10   1.10500     8910.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     H_rad
sSPC(1474)+H=tSPC(3683)+H2 2.2757168e+06   2.31000     4947.50000
!H_Abstraction estimate: (Average:)  C/H3/CO     H_rad
sSPC(1474)+H=sSPC(1356)+H2 1.0634848e+10   1.10500     8910.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     H_rad
sSPC(3121)+H=sSPC(3071)+H2 1.0634848e+10   1.10500     8910.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     H_rad
H+tSPC(346)=H2+H2CCCO 7.7460197e+12        -0.06091    -63.81982
!Disproportionation estimate: (Average:)  H_rad     COpri_Cdrad
H+C3H3O-enone=H2+H2CCCO 5.4132535e+12      -0.08875    -36.56250
!Disproportionation estimate: (Average:)  H_rad     Cdpri_COrad
HOC[CH2][CH3]2+C4H8O2(62)=tBuOH+tSPC(54) 1.4867217e+03       2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
O/H/NonDeO
iC4H7+C4H8O2(62)=iC4H8+tSPC(54) 1.4867217e+03    2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cd     O/H/NonDeO
tSPC(54)+HO2=C4H8O2(62)+O2 1.7500000e+10   0.00000     -3275.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO     O_Orad
HOC[CH2][CH3]2+C4H8O2(62)=tBuOH+tSPC(77) 1.6800000e+12       0.00000
12400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
iC4H8+tSPC(77)=iC4H7+C4H8O2(62) 3.4680000e+13    0.00000     21400.00000
       !H_Abstraction exact:   C_rad/H2/Cd     C/H3/Cd
OH+C4H8O2(62)=H2O+tSPC(77) 3.4482017e+07   1.75000     3789.37500
!H_Abstraction estimate: (Average:)  O_pri_rad     C/H3/Cd
tSPC(77)+HO2=C4H8O2(62)+O2 3.0000000e+11   0.00000     0.00000
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     O_Orad
!CH2C[O]CH3+C4H8O2(62)=H2CCCH3[OH]+tSPC(54) 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH2C[O]CH3+C4H8O2(62)=H2CCCH3[OH]+tSPC(54)      6.99e-02 3.75 10.89e+03
!MHS 04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
H2CCCH3[OH]+tSPC(77)=CH2C[O]CH3+C4H8O2(62) 1.4867217e+03     2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cd
CH3+C4H8O2(62)=CH4+tSPC(54) 1.4867217e+03        2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  C_methyl     O/H/NonDeO
CH3+C4H8O2(62)=CH4+tSPC(77) 2.4120000e+02        2.92000     7160.00000
       !H_Abstraction exact:   C/H3/Cd     C_methyl
CH2O+tSPC(54)=HCO+C4H8O2(62) 4.1200000e+04       2.50000     10210.00000
       !H_Abstraction exact:   CO_pri     O_rad/NonDeO
CH2O+tSPC(77)=HCO+C4H8O2(62) 5.5000000e+03       2.81000     5860.00000
       !H_Abstraction estimate: (Average:)  CO_pri     C_rad/H2/Cd
tSPC(54)+tSPC(346)=C4H8O2(62)+H2CCCO 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Cdrad
tSPC(77)+tSPC(346)=C4H8O2(62)+H2CCCO 7.7460197e+12     -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  C_rad/H2/Cd
COpri_Cdrad
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tSPC(54)+C3H3O-enone=C4H8O2(62)+H2CCCO 5.4132535e+12   -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  O_rad/NonDeO
Cdpri_COrad
tSPC(77)+C3H3O-enone=C4H8O2(62)+H2CCCO 5.4132535e+12   -0.08875    -
36.56250     !Disproportionation estimate: (Average:)  C_rad/H2/Cd
Cdpri_COrad
tSPC(1286)+C4H8O2(62)=tSPC(1416)+tSPC(54) 1.7300000e+01      3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/NonDeO
tSPC(1286)+C4H8O2(62)=tSPC(1416)+tSPC(77) 3.4482017e+07      1.75000
3789.37500   !H_Abstraction estimate: (Average:)  O_rad/NonDeO
C/H3/Cd
tSPC(54)+CH2CHO=C4H8O2(62)+CH2CO 5.4132535e+12   -0.08875    -36.56250
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cdpri_Orad
tSPC(77)+CH2CHO=C4H8O2(62)+CH2CO 5.4132535e+12   -0.08875    -36.56250
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cdpri_Orad
!CH2CHO+C4H8O2(62)=C2H4O+tSPC(54) 1.7300000e+01        3.40000     -
1140.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
O/H/NonDeO
CH2CHO+C4H8O2(62)=C2H4O+tSPC(54)    6.99e-02 3.75 10.89e+03  !MHS
04/29/11 (CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
CH2CHO+C4H8O2(62)=C2H4O+tSPC(77) 3.4482017e+07   1.75000     3789.37500
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     C/H3/Cd
sSPC(1735)+tSPC(54)=sSPC(1697)+C4H8O2(62) 1.7300000e+01      3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/NonDeO
O_rad/NonDeO
sSPC(1735)+tSPC(77)=sSPC(1697)+C4H8O2(62) 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/NonDeO
C_rad/H2/Cd
tSPC(54)+CH3O=C4H8O2(62)+CH2O 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Orad
tSPC(77)+CH3O=C4H8O2(62)+CH2O 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cmethyl_Orad
H2O2+tSPC(54)=HO2+C4H8O2(62) 3.4600000e+01       3.40000     -1140.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     O_rad/NonDeO
H2O2+tSPC(77)=HO2+C4H8O2(62) 2.9734435e+03       2.38600     9690.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeO     C_rad/H2/Cd
tSPC(3683)+C4H8O2(62)=sSPC(1474)+tSPC(54) 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/CO
O/H/NonDeO
sSPC(1474)+tSPC(77)=sSPC(1356)+C4H8O2(62) 1.4867217e+03      2.38600
9690.00000   !H_Abstraction estimate: (Average:)  O/H/NonDeO
C_rad/H2/Cd
tSPC(54)+CH3CO=C4H8O2(62)+CH2CO 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_COrad
tSPC(77)+CH3CO=C4H8O2(62)+CH2CO 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cmethyl_COrad
sSPC(3071)+C4H8O2(62)=sSPC(3121)+tSPC(54) 1.7300000e+01      3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O_rad/NonDeO
O/H/NonDeO
sSPC(3071)+C4H8O2(62)=sSPC(3121)+tSPC(77) 3.4482017e+07      1.75000
3789.37500   !H_Abstraction estimate: (Average:)  O_rad/NonDeO
C/H3/Cd
tSPC(54)+sSPC(2810)=C4H8O2(62)+CO2 7.7460197e+12       -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Orad
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H+C4H8O2(62)=H2+tSPC(54) 1.0634848e+10     1.10500     8910.00000
!H_Abstraction estimate: (Average:)  H_rad     O/H/NonDeO
H+C4H8O2(62)=H2+tSPC(77) 1.2990000e+06     2.38000     2800.00000
!H_Abstraction exact:   C/H3/Cd     H_rad
tSPC(77)+C4H8O2(62)=C4H8O2(62)+tSPC(54) 1.4867217e+03        2.38600
9690.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/NonDeO
C4H8O2(62)+O=tSPC(77)+OH 2.5650000e+04     3.05000     3123.00000
!H_Abstraction estimate: (Average:)  C/H3/Cd     O_atom_triplet
C4H8O2(62)+O=tSPC(54)+OH 1.0000000e+13     0.00000     4690.00000
!H_Abstraction estimate: (Average:)  O/H/NonDeO     O_atom_triplet
C4H7OJ(79)+HO2=tSPC(110)+H2O2 2.8000000e+04      2.69000     11300.00000
       !H_Abstraction estimate: (Average:)  X_H     O_rad/NonDeO
C4H7OJ(79)+iC4H7=tSPC(110)+iC4H8 9.4533885e+08   1.22646     13808.35399
       !H_Abstraction estimate: (Average:)  X_H     C_rad/H2/Cd
C4H7OJ(79)+tSPC(54)=tSPC(110)+C4H8O2(62) 2.8000000e+04       2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/NonDeO
C4H7OJ(79)+tSPC(77)=tSPC(110)+C4H8O2(62) 9.4533885e+08       1.22646
13808.35399        !H_Abstraction estimate: (Average:)  X_H
C_rad/H2/Cd
C4H7OJ(79)+OH=tSPC(110)+H2O 2.4000000e+06        2.00000     10100.00000
       !H_Abstraction exact:   X_H     O_pri_rad
C4H7OJ(79)+HOC[CH2][CH3]2=tSPC(110)+tBuOH 9.4533885e+08      1.22646
13808.35399        !H_Abstraction estimate: (Average:)  X_H
C_rad/H2/Cs
C4H7OJ(79)+CH3=tSPC(110)+CH4 1.6200000e+06       1.87000     13000.00000
       !H_Abstraction exact:   X_H     C_methyl
C4H7OJ(79)+sSPC(1697)=tSPC(110)+sSPC(1735) 2.8000000e+04     2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/NonDeO
C4H7OJ(79)+tSPC(1286)=tSPC(110)+tSPC(1416) 2.8000000e+04     2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/NonDeO
C4H7OJ(79)+CH2CHO=tSPC(110)+C2H4O 2.8000000e+04        2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/OneDe
C4H7OJ(79)+CH2C[O]CH3=tSPC(110)+H2CCCH3[OH] 2.8000000e+04    2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/OneDe
C4H7OJ(79)+sSPC(1356)=tSPC(110)+sSPC(1474) 2.8000000e+04     2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/NonDeO
C4H7OJ(79)+tSPC(3683)=tSPC(110)+sSPC(1474) 9.4533885e+08     1.22646
13808.35399        !H_Abstraction estimate: (Average:)  X_H
C_rad/H2/CO
C4H7OJ(79)+sSPC(3071)=tSPC(110)+sSPC(3121) 2.8000000e+04     2.69000
11300.00000        !H_Abstraction estimate: (Average:)  X_H
O_rad/NonDeO
C4H7OJ(79)+H=tSPC(110)+H2 4.8000000e+08    1.50000     9400.00000
!H_Abstraction exact:   X_H     H_rad
HO2+tSPC(110)=O2+C4H7OJ(79) 3.0000000e+11        0.00000     0.00000
!Disproportionation exact:   O_Orad     Y_rad
CH3O+tSPC(110)=CH2O+C4H7OJ(79) 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Orad     Y_rad
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!C3H3O-enone+tSPC(110)=H2CCCO+C4H7OJ(79) 5.4132535e+12       -0.08875
-36.56250    !Disproportionation estimate: (Average:)  Cdpri_Csrad
Y_rad
tSPC(110)+C3H3O-enone=C4H7OJ(79)+H2CCCO   3.489111451440034E12    -0.071
      2.68075e+03 !Disproportionation estimate: (Average:)  Y_rad
Cdpri_Csrad       deltaHrxn(T=298K) = -3.8696366309089214 kcal/mol
!tSPC(346)+tSPC(110)=H2CCCO+C4H7OJ(79) 7.7460197e+12   -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Cdrad
Y_rad
tSPC(110)+tSPC(346)=C4H7OJ(79)+H2CCCO     5.298533849488731E12    -
0.04569761904761904     0.31545783730158733e+03 !Disproportionation
estimate: (Average:)    Y_rad     COpri_Cdrad         deltaHrxn(T=298K)
= -25.797311660771186 kcal/mol
CH3CO+tSPC(110)=CH2CO+C4H7OJ(79) 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_COrad     Y_rad
CH2CHO+tSPC(110)=CH2CO+C4H7OJ(79) 7.7460197e+12        -0.06091    -
63.81982     !Disproportionation estimate: (Average:)  COpri_Csrad
Y_rad

tBuOH+O=OC[CH3]3+OH           1.0E13      0.0   4.69e+03
      !H_Abstraction exact:   O/H/NonDeC     O_atom_triplet
OC[CH3]3+H2O2=tBuOH+HO2       34.6        3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeO
HO2+OC[CH3]3=O2+tBuOH         1.75E10     0.0   -3.275e+03
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/NonDeC

!H-abstractions of C5H10_iso
C5H9J(5)+H2=C5H10_iso+H       8.98E12     0.0   10.3e+03
      !H_Abstraction exact:   H2     Cd_pri_rad
C5H10_iso+H=C5H9J(7)+H2       1.299E6     2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad
C5H10_iso+H=C5H9J(8)+H2       1.398E6     2.36  1.11e+03
      !H_Abstraction exact:   C/H2/OneDeC     H_rad
C5H9J(9)+H2=C5H10_iso+H       9.14E11     0.0   14.8e+03
      !H_Abstraction exact:   H2     C_rad/H2/Cs
C5H9J(5)+CH4=C5H10_iso+CH3    6.36E14     0.0   13.7e+03
      !H_Abstraction exact:   C_methane     Cd_pri_rad
C5H10_iso+CH3=C5H9J(7)+CH4    241.2       2.92  7.16e+03
      !H_Abstraction exact:   C/H3/Cd     C_methyl
C5H10_iso+CH3=C5H9J(8)+CH4    5.46E13     0.0   10.4e+03
      !H_Abstraction exact:   C/H2/OneDeC     C_methyl
C5H10_iso+CH3=C5H9J(9)+CH4    834000.0    1.9   11.05e+03
      !H_Abstraction exact:   C/H3/Cs     C_methyl
C5H10_iso+OH=C5H9J(5)+H2O     1.026E13    0.0   5.94e+03
      !H_Abstraction exact:   Cd_pri     O_pri_rad
C5H10_iso+OH=C5H9J(7)+H2O     3.448E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
C5H10_iso+OH=C5H9J(8)+H2O     3.173E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_pri_rad
C5H10_iso+OH=C5H9J(9)+H2O     3600000.0   2.0   0.86e+03
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
C5H9J(5)+iC4H8=C5H10_iso+iC4H7      4.638E13    0.0   7.5e+03
      !H_Abstraction exact:   C/H3/Cd     Cd_pri_rad
C5H9J(7)+iC4H8=C5H10_iso+iC4H7      3.468E13    0.0   21.4e+03
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C5H10_iso+iC4H7=C5H9J(8)+iC4H8      3.040E6     1.886 9.448e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     C_rad/H2/Cd
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C5H9J(9)+iC4H8=C5H10_iso+iC4H7      3.36E12     0.0   12.4e+03
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs

!Beta-scissions of C5H9J radicals
C4H6-1+CH3=C5H9J(5)     1.99E13     0.0   12.1e+03
      !R_Addition_MultipleBond exact:     Ct/Nd_Ct/H     C_methyl
pC3H4+C2H5=C5H9J(5)     1.999E10    0.0   6.975e+03
      !R_Addition_MultipleBond estimate: (Average:)   Ct/Nd_Ct/H
C_rad/H2/Cs
aC3H4+C2H5=C5H9J(7)     3.853E11    0.041 9.29e+03
      !R_Addition_MultipleBond estimate: (Average:)   Ca_Cd/H2
C_rad/H2/Cs
C4H6-12+CH3=C5H9J(8)    1.58E11     0.0   4.97e+03
      !R_Addition_MultipleBond exact:     Ca_Cd/H2     C_methyl
sC3H5+C2H4=C5H9J(9)     1.448E13    0.0   4.5e+03
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H2     Cd_rad/NonDe

!Isomerizations of C5H9J radicals
C5H9J(5)=C5H9J(7) 1.53E10     0.97  37.7e+03    !intra_H_migration
exact:      R3H_DS     Cd_rad_out_singleH     Cs_H_out_2H
C5H9J(5)=C5H9J(8) 1.846E10    0.74  34.7e+03    !intra_H_migration
exact:      R3H_DS     Cd_rad_out_singleH     Cs_H_out_H/NonDeC
C5H9J(5)=C5H9J(9) 6.143E8     1.138 34.79e+03   !intra_H_migration
estimate: (Average:)    R4H_DSS     Cd_rad_out_singleH     Cs_H_out_2H
C5H9J(7)=C5H9J(8) 8.4E10      0.82  49.2e+03    !intra_H_migration
exact:      R3H_SS_2Cd     C_rad_out_2H     Cs_H_out_H/NonDeC
C5H9J(9)=C5H9J(7) 7.62E9      0.35  19.76e+03   !intra_H_migration
estimate: (Average:)    R4H_SSS     C_rad_out_2H     Cs_H_out_2H
C5H9J(9)=C5H9J(8) 2.82E8      1.28  27.9e+03    !intra_H_migration
exact:      Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe

!CH3 addition to iC4H8
iC4H8+CH3=C5H11J(10)    3.99E12     0.0   8.0e+03
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/Nd2     C_methyl

!H addition to C5H10_iso
C5H10_iso+H=C5H11J(10)  4.94E13     0.0   1.5e+03
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/Nd2     H_rad
C5H10_iso+H=C5H11J(11)  1.17E13     0.0   4.7e+03
      !R_Addition_MultipleBond exact:     Cd/Nd2_Cd/H2     H_rad

!Beta-scissions of C5H11J(11)
C4H8-1+CH3=C5H11J(11)   1.36E12     0.0   10.1e+03
      !R_Addition_MultipleBond exact:     Cd/H/Nd_Cd/H2     C_methyl
C3H6+C2H5=C5H11J(11)    2.483E10    0.244 10.4875e+03
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/H2
C_rad/H2/Cs

!New rxns from C5H10_iso RMG run
C5H8(95)+H=C5H9J(8) 3.7100000e+13    0.00000     1000.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/H/De     H_rad
CH3+C5H9J(8)=CH4+C5H8(95) 6.5700000e+14    -0.68000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_methyl
C5H9J(8)+C5H9J(8)=C5H10_iso+C5H8(95) 6.3300000e+14     -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
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H+C5H9J(8)=H2+C5H8(95) 1.0830000e+13       0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     H_rad
C5H11J(10)+C5H9J(8)=C5H10_iso+C5H10_iso 1.2660000e+15        -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
C5H11J(10)+CH3=C5H10_iso+CH4 1.3140000e+15       -0.68000    0.00000
!Disproportionation exact:   C_methyl     Cmethyl_Csrad
C5H11J(10)+H=C5H10_iso+H2 2.1660000e+13    0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
iC4H7+C5H9J(8)=iC4H8+C5H8(95) 6.8700000e+13      -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
iC4H7+C5H11J(10)=iC4H8+C5H10_iso 1.3740000e+14   -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C5H11J(10)+C5H9J(9)=C5H10_iso+C5H10_iso 1.3800000e+14        -0.35000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
C5H9J(9)+C5H10_iso=C5H10_iso+C5H9J(8) 3.0397882e+06    1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C_rad/H2/Cs
C/H2/OneDeC
C5H8(95)+H=C5H9J(9) 2.8500000e+13    0.00000     4300.00000
!R_Addition_MultipleBond exact:   Cd/H/De_Cd/H2     H_rad
C5H9J(9)+C5H9J(8)=C5H8(95)+C5H10_iso  5.7005859e+12    -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/De_Csrad
C_rad/H/OneDeC
DUP
C5H9J(9)+C5H9J(8)=C5H8(95)+C5H10_iso  2.3000000e+13    -0.35000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
DUP
C5H9J(9)+C5H9J(9)=C5H8(95)+C5H10_iso 1.1401172e+13     -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/De_Csrad
C_rad/H2/Cs
C5H9J(9)+CH3=C5H8(95)+CH4 1.1401172e+13    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     C_methyl
C5H9J(9)+H=C5H8(95)+H2 1.1401172e+13       -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     H_rad
C5H9J(9)+iC4H7=C5H8(95)+iC4H8 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     C_rad/H2/Cd
!sC3H5+C5H9J(9)=C8H14 1.4157154e+13        -0.15000    291.66667
!R_Recombination estimate: (Average:)  Cd_rad/NonDe     C_rad/H2/Cs
C2H5+C5H9J(8)=C2H4+C5H10_iso 6.3300000e+14       -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
C2H5+C5H9J(9)=C2H4+C5H10_iso 6.9000000e+13       -0.35000    0.00000
!Disproportionation exact:   C_rad/H2/Cs     Cmethyl_Csrad
C2H5+iC4H7=C2H4+iC4H8 6.8700000e+13        -0.35000    -130.00000
!Disproportionation exact:   C_rad/H2/Cd     Cmethyl_Csrad
CH3+sC3H5=CH4+aC3H4 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_methyl     Cmethyl_Cdrad
iC4H7+sC3H5=iC4H8+aC3H4 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cd     Cmethyl_Cdrad
C5H9J(8)+sC3H5=C5H10_iso+aC3H4 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Cdrad
H+sC3H5=H2+aC3H4 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  H_rad     Cmethyl_Cdrad
C5H9J(9)+sC3H5=C5H10_iso+aC3H4 7.0652342e+13     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H2/Cs     Cmethyl_Cdrad
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pC3H3+iC4H8=pC3H4+iC4H7 1.5480000e+13      0.00000     18200.00000
!H_Abstraction exact:   C/H3/Cd     C_rad/H2/Ct

pC3H3+C5H10_iso=pC3H4+C5H9J(8) 3.0397882e+06     1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Ct     C/H2/OneDeC
pC3H4+C5H9J(9)=pC3H3+C5H10_iso 9.4074532e+06     1.75273     12532.12121
       !H_Abstraction estimate: (Average:)  C/H3/Ct     C_rad/H2/Cs
!pC3H3+H=pC3H4 5.0000000e+13   0.00000     0.00000     !R_Recombination
estimate: (Average:)  C_rad/H2/Ct     H_rad
C5H11J(10)+pC3H3=C5H10_iso+pC3H4 6.9019473e+13   -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/Ct
C5H9J(9)+pC3H3=C5H8(95)+pC3H4 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     C_rad/H2/Ct
C5H9J(8)+pC3H3=C5H8(95)+pC3H4 3.4509736e+13      -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/Ct
C2H5+pC3H3=C2H4+pC3H4 3.4509736e+13        -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/Ct
aC3H4+iC4H7=pC3H3+iC4H8 2.1440000e+14      0.00000     30700.00000
!H_Abstraction exact:   C_rad/H2/Cd     Cd_pri
pC3H3+C5H10_iso=aC3H4+C5H9J(8) 1.0200000e+03     3.10000     8820.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H2/OneDeC
aC3H4+C5H9J(9)=pC3H3+C5H10_iso 3.1280000e+13     0.00000     19700.00000
       !H_Abstraction exact:   Cd_pri     C_rad/H2/Cs
C5H11J(10)+pC3H3=C5H10_iso+aC3H4 9.1200000e+14   -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C5H9J(9)+pC3H3=C5H8(95)+aC3H4 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/De_Csrad     Cd_pri_rad
C5H9J(8)+pC3H3=C5H8(95)+aC3H4 4.5600000e+14      -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C2H5+pC3H3=C2H4+aC3H4 4.5600000e+14        -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
sC3H5+pC3H3=aC3H4+pC3H4 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Cdrad     C_rad/H2/Ct
sC3H5+pC3H3=aC3H4+aC3H4 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Cdrad     Cd_pri_rad
aC3H4+pC3H3=pC3H3+pC3H4 1.0200000e+14      0.00000     26800.00000
!H_Abstraction exact:   Cd_pri     C_rad/H2/Ct
C5H10_iso+pC3H3=SPC(482) 7.2990714e+11     0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/Nd2_Cd/H2
Y_rad_birad
C5H10_iso+pC3H3=SPC(483) 7.2990714e+11     0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/Nd2
Y_rad_birad
C2H4+pC3H3=C5H7J(504) 1.4598143e+12        0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/H2
Y_rad_birad
C5H8(95)+pC3H3=SPC(493) 7.2990714e+11      0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/Nd/De_Cd/H2
Y_rad_birad
C5H8(95)+pC3H3=SPC(494) 7.2990714e+11      0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/De_Cd/H2
Y_rad_birad
C5H8(95)+pC3H3=SPC(495) 7.2990714e+11      0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/H/De
Y_rad_birad
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C5H8(95)+pC3H3=SPC(496) 7.2990714e+11      0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/Nd/De
Y_rad_birad
iC4H8+pC3H3=SPC(498) 7.2990714e+11   0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/Nd2
Y_rad_birad
iC4H8+pC3H3=SPC(499) 7.2990714e+11   0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/Nd2_Cd/H2
Y_rad_birad
aC3H4+pC3H3=C6H7J(511) 1.4598143e+12       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Ca_Cd/H2     Y_rad_birad
aC3H4+pC3H3=C6H7J(512) 1.4598143e+12       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Ca     Y_rad_birad
pC3H4+pC3H3=C6H7J(505) 7.2990714e+11       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Ct/Nd_Ct/H
Y_rad_birad
C6H7J(505)=C6H7J(511) 1.5300000e+10        0.97000     37700.00000
!intra_H_migration exact:   R3H_DS     Cd_rad_out_singleH
Cs_H_out_2H
pC3H4+pC3H3=C6H7J(506) 7.2990714e+11       0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Ct/H_Ct/Nd
Y_rad_birad
C*C*CC*C*C+H=C6H7J(512) 3.7666519e+13      0.00000     2900.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H/De_Ca     H_rad
CH3+C6H7J(512)=CH4+C*C*CC*C*C 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C_methyl     C/H2/De_Cdrad
iC4H7+C6H7J(512)=iC4H8+C*C*CC*C*C 1.1401172e+13        -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H2/Cd
C/H2/De_Cdrad
C5H9J(8)+C6H7J(512)=C5H10_iso+C*C*CC*C*C 1.1401172e+13       -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H2/De_Cdrad
H+C6H7J(512)=H2+C*C*CC*C*C 1.1401172e+13   -0.07100    -2.16667
!Disproportionation estimate: (Average:)  H_rad     C/H2/De_Cdrad
C5H9J(9)+C6H7J(512)=C5H10_iso+C*C*CC*C*C 1.1401172e+13       -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/De_Cdrad
pC3H3+C6H7J(512)=pC3H4+C*C*CC*C*C 1.1401172e+13        -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H2/Ct
C/H2/De_Cdrad
pC3H3+C6H7J(512)=aC3H4+C*C*CC*C*C 1.1401172e+13        -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  Cd_pri_rad
C/H2/De_Cdrad
C*C*CC*C*C+H=C6H7J(506) 1.3360000e+14      0.00000     2900.00000
!R_Addition_MultipleBond exact:   Cd/H2_Ca     H_rad
CH3+C6H7J(506)=CH4+C*C*CC*C*C 7.0652342e+13      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_methyl     Cmethyl_Cdrad
iC4H7+C6H7J(506)=iC4H8+C*C*CC*C*C 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  C_rad/H2/Cd
Cmethyl_Cdrad
C5H9J(8)+C6H7J(506)=C5H10_iso+C*C*CC*C*C 7.0652342e+13       -0.22972
-1.80556     !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Cdrad
H+C6H7J(506)=H2+C*C*CC*C*C 7.0652342e+13   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  H_rad     Cmethyl_Cdrad
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C5H9J(9)+C6H7J(506)=C5H10_iso+C*C*CC*C*C 7.0652342e+13       -0.22972
-1.80556     !Disproportionation estimate: (Average:)  C_rad/H2/Cs
Cmethyl_Cdrad
pC3H3+C6H7J(506)=pC3H4+C*C*CC*C*C 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  C_rad/H2/Ct
Cmethyl_Cdrad
pC3H3+C6H7J(506)=aC3H4+C*C*CC*C*C 7.0652342e+13        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cd_pri_rad
Cmethyl_Cdrad


!New rxns from C8H14 RMG run
C8H14+iC4H7=C8H13J(41)+iC4H8 6.0795764e+06       1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C/H2/OneDeC     C_rad/H2/Cd
C5H8(95)+sC3H5=C8H13J(41) 7.2400000e+12    0.00000     4500.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/H/De
Cd_rad/NonDe
!C8H13J(41)+H=C8H14 5.0000000e+13    0.00000     0.00000
!R_Recombination estimate: (Average:)  C_rad/H/OneDeC     H_rad
C8H15J(44)+C8H13J(41)=C8H14+C8H14 1.2660000e+15        -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeC
!iC4H8+iC4H7=C8H15J(44) 5.0381048e+11      0.00000     15645.00000
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/Nd2
C_rad/H2/Cd
C8H15J(44)+iC4H7=C8H14+iC4H8 1.3740000e+14       -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
!C8H14+H=C8H15J(44) 9.8800000e+13    0.00000     1500.00000
!R_Addition_MultipleBond exact:   Cd/H2_Cd/Nd2     H_rad
C8H14+H=C8H13J(41)+H2 2.7960000e+06        2.36000     1110.00000
!H_Abstraction exact:   C/H2/OneDeC     H_rad
H+C8H15J(44)=H2+C8H14 2.1660000e+13        0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     H_rad
C8H13J(41)+sC3H5=C8H14+aC3H4 7.0652342e+13       -0.22972    -1.80556
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Cdrad
C8H14+CH3=C8H13J(41)+CH4 1.0920000e+14     0.00000     10400.00000
!H_Abstraction exact:   C/H2/OneDeC     C_methyl
CH3+C8H15J(44)=CH4+C8H14 1.3140000e+15     -0.68000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_methyl
pC3H3+C8H14=pC3H4+C8H13J(41) 6.0795764e+06       1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Ct     C/H2/OneDeC
C8H15J(44)+pC3H3=C8H14+pC3H4 6.9019473e+13       -0.23333    -43.33333
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     C_rad/H2/Ct
pC3H3+C8H14=aC3H4+C8H13J(41) 2.0400000e+03       3.10000     8820.00000
       !H_Abstraction estimate: (Average:)  Cd_pri_rad     C/H2/OneDeC
C8H15J(44)+pC3H3=C8H14+aC3H4 9.1200000e+14       -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C8H14+pC3H3=SPC(425) 1.4598143e+12   0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/Nd2_Cd/H2
Y_rad_birad
C8H14+pC3H3=SPC(426) 1.4598143e+12   0.17975     2985.07963
!R_Addition_MultipleBond estimate: (Average:)  Cd/H2_Cd/Nd2
Y_rad_birad
C8H13J(41)+C6H7J(512)=C8H14+C*C*CC*C*C 1.1401172e+13   -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H2/De_Cdrad
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pC3H3+iC4H7=C7H10(454) 1.1500000e+13       0.00000     0.00000
!R_Recombination estimate: (Average:)  C_rad/H2/Ct     C_rad/H2/Cd
C6H7J(506)+C8H13J(41)=C*C*CC*C*C+C8H14 7.0652342e+13   -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Cdrad
C_rad/H/OneDeC

!C4H6-13+OH=C4H7O-13    5.42E12     0.0   0.0
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H2_Cd/H/De
O_pri_rad

!CH3CHCHCHO+H=C4H7O_1_2 7.299E11    0.180 2.985e+03
      !R_Addition_MultipleBond estimate: (Average:)   OCO     H_rad
CH3+CHCHCHO=CH3CHCHCHO  7.23E13     0.0   0.0         !R_Recombination
exact:      Cd_pri_rad     C_methyl
pC3H5+HCO=CH3CHCHCHO    1.81E13     0.0   0.0         !R_Recombination
exact:      CO_pri_rad     Cd_pri_rad
C3H6+CO=CH3CHCHCHO      8.0834E7    1.70  82.775e+03  !1,2_Insertion
estimate: (Average:)    Cd_pri     CO_birad

C2H2+HCO=CHCHCHO        1.04E12     0.0   6.56e+03
      !R_Addition_MultipleBond estimate: (Average:)   Ct/H_Ct/H
CO_pri_rad
!C2H3+CO=CHCHCHO        8.0834E7    1.70  82.775e+03  !1,2_Insertion
exact:      CO_birad     R_H

O2+C4H9O-4=HO2+nC4H8O  4.6826e+11 0.3321 -1.0635e+03 !from Zador et al
calculated for CH3CHOH+O2=HO2+CH3CHO (consistent with RMG) (edited by
MHS 04.27.11)
!O2+C4H9O-4=HO2+nC4H8O  2.28E12     0.0   0.0
      !Disproportionation_O2d exact:      O2d     O_Csrad

!CBS-QB3 calculations (w/o HR corrections)
C4H9O-1+H2O2=HO2+nC4H10O      5.76e+00    3.16  0.75e+03
C4H9O-2+H2O2=HO2+nC4H10O      1.35e+00    3.42  1.43e+03
C4H9O-3+H2O2=HO2+nC4H10O      6.29e-01    3.52  1.61e+03
C4H9O-4+H2O2=HO2+nC4H10O      2.97e+00    3.39  1.40e+03

!C4H7OJ(16)+H2O2=nC4H8O+HO2   2973.44     2.386 9.69e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     O/H/NonDeO
!C4H7OJ(13)+H2O2=nC4H8O+HO2   2973.44     2.386 9.69e+03
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     O/H/NonDeO
!C4H7OJ(12)+H2O2=nC4H8O+HO2   2973.44     2.386 9.69e+03
      !H_Abstraction estimate: (Average:) C_rad/H/OneDeC     O/H/NonDeO
!CBS-QB3 calculations (w/o HR correction)
!C4H7OJ(16)+H2O2=nC4H8O+HO2   6.14e-01    3.51  1.58e+03
!C4H7OJ(13)+H2O2=nC4H8O+HO2   2.31e-01    3.62  1.75e+03
!C4H7OJ(12)+H2O2=nC4H8O+HO2   2.26e-02    3.89  6.77e+03
!New estimates, based on nBuOH+HO2
C4H7OJ(16)+H2O2=nC4H8O+HO2    5.76e+00    3.16  0.75e+03
C4H7OJ(13)+H2O2=nC4H8O+HO2    1.35e+00    3.42  1.43e+03
nC4H8O+HO2=H2O2+C4H7OJ(12)    1.00e+12    0.00  14000.96    !Based on
CH3CHO+HO2=H2O2+CH2CHO

!nC4H8O+OH=H2O+C4H7OJ(12)     2.26e+02    3.07  -2.32e+03
nC4H8O+OH=H2O+C4H7OJ(12)      1.60e+13    0           2000.48 !Estimate,
based on CH3CHO+OH=H2O+CH2CHO
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!HO2+C4H7OJ(16)=O2+nC4H8O     3.0E11      0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs
!HO2+C4H7OJ(13)=O2+nC4H8O     3.0E11      0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/NonDeC
!HO2+C4H7OJ(12)=O2+nC4H8O     3.0E11      0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad
C_rad/H/OneDeC

!C3H6O+H=HOCHC2H5 7.3E11      0.18  2985.08     !R_Addition_MultipleBond
estimate: (Average:)    OCO     H_rad

C2H4O+HO2=H2O2+CH2CHO   1.00e+12    0.0   14000.0
C4H8-1+HO2=H2O2+C4H7-24 9.62e+03    2.6   13910.0
C4H6-13+OH=H2O+nC4H5    2.052e13    0.0   5.94e+03
!C4H6-13+OH=H2O+iC4H5   2.22e6      2.0   1.45e+03

nC4H10O+O2=C4H9O-1+HO2  1.206E14    0.0   51.87e+03   !H_Abstraction
exact:      C/H3/Cs     O2b
nC4H10O+O2=C4H9O-2+HO2  1.588E14    0.0   47.69e+03   !H_Abstraction
exact:      C/H2/NonDeC     O2b
nC4H10O+O2=C4H9O-3+HO2  1.588E14    0.0   47.69e+03   !H_Abstraction
exact:      C/H2/NonDeC     O2b
nC4H10O+O2=C4H9O-4+HO2  1.588E14    0.0   47.69e+03   !H_Abstraction
estimate: (Average:)    C/H2/CsO     O2b
nC4H10O+O2=C4H9O-5+HO2  2.325E12    0.0   74.12e+03   !H_Abstraction
estimate: (Average:)    O/H/NonDeC     O2b

nC4H8O+O2=C4H7OJ(16)+HO2      1.206E14    0.0   51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b
nC4H8O+O2=C4H7OJ(13)+HO2      1.588E14    0.0   47.69e+03
      !H_Abstraction exact:   C/H2/NonDeC     O2b
nC4H8O+O2=C4H7OJ(12)+HO2      1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O2b
nC4H8O+O2=C4H7OJ(8)+HO2 1.204E14    0.0   39.15e+03   !H_Abstraction
exact:      CO/H/NonDe     O2b

!H-abstraction by O2(triplet) instead of O2(singlet)
!sBuOH+O2=CH2CH[OH]C2H5+HO2          1.206E14    0.0         51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b
!sBuOH+O2=CH3C[OH]C2H5+HO2          1.588E14    0.0         43.92e+03
      !H_Abstraction estimate: (Average:) C/H/NDMustO     O2b
!sBuOH+O2=CH3CH[OH]CHCH3+HO2        1.588E14    0.0         47.69e+03
      !H_Abstraction exact:   C/H2/NonDeC     O2b
!sBuOH+O2=CH3CH[OH]CH2CH2+HO2 1.206E14    0.0         51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b
!sBuOH+O2=CH3CH[O]C2H5+HO2          674422.1    2.106 16.1634e+03
      !H_Abstraction estimate: (Average:) O/H/NonDeC     O2b
!tBuOH+O2=OC[CH3]3+HO2              674422.1    2.106 16.1634e+03
      !H_Abstraction estimate: (Average:) O/H/NonDeC     O2b
!tBuOH+O2=HOC[CH2][CH3]2+HO2        3.618E14    0.0         51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b

!CBS-QB3 calculations w/o HR corrections
CH2CH[OH]C2H5+H2O2=HO2+sBuOH  6.11e-01    3.53   1.52e+03
CH3C[OH]C2H5+H2O2=HO2+sBuOH         3.46e+01    3.05   1.02e+03
CH3CH[OH]CHCH3+H2O2=HO2+sBuOH 1.75e+00    2.91  -0.41e+03
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CH3CH[OH]CH2CH2+H2O2=HO2+sBuOH      1.15e+01    2.94   0.46e+03
HOC[CH2][CH3]2+H2O2=HO2+tBuOH 4.20e-01    3.53   1.56e+03

!
!ISOBUTANOL
!
!Updated by MRH on 11/JUN/2010 (cbs-qb3 calculations w/1D hindered rotor
corrections) original
iBuOH+H=H2+C4H9Oi1      2.19e+06    2.22  8.46e+03
iBuOH+H=H2+C4H9Oi2      1.00e+06    2.13  4.29e+03
iBuOH+H=H2+C4H9Oi3      1.05e+06    2.20  3.96e+03
iBuOH+H=H2+C4H9Oi4      4.05e+04    2.38  9.34e+03

iBuOH+OH=H2O+C4H9Oi1    1.05E+06    1.9   860.0 !H_Abstraction exact:
      C/H3/Cs     O_pri_rad
!iBuOH+OH=H2O+C4H9Oi2   3.90E+06    1.9   360.0       !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad
!The following comes from: W. Tsang, "Chemical kinetic database for
comubstion chemistry.  Part IV.  Isobutane"
!     J. Phys. Chem. Ref. Data. 19 (1990) 1-68
!The kinetic rate is for iso-butane + OH = H2O + tert-C4H9
!iBuOH+OH=H2O+C4H9Oi2   5.73E+10    0.51  64.532
iBuOH+OH=H2O+C4H9Oi2    0.72E+10    0.51  64.532
iBuOH+OH=H2O+C4H9Oi3    0.90E+06    1.9   1160.0
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_pri_rad
!iBuOH+OH=H2O+C4H9Oi3   3.90E+06    1.9   160.0       !H_Abstraction
estimate: (Average:)    C/H2/CsO     O_pri_rad
iBuOH+OH=H2O+C4H9Oi4    1.23E+10    0.30  1834.0      !EtOH Marinov 1998


!CBS-QB3 calculations w/1DHR corrections
!iBuOH+CH3=CH4+C4H9Oi1  6.62e+01    3.38  9.88e+03
!iBuOH+CH3=CH4+C4H9Oi2  2.40e+01    3.24  8.06e+03
iBuOH+CH3=CH4+C4H9Oi3   1.53e+01    3.11  6.95e+03
!iBuOH+CH3=CH4+C4H9Oi4  1.87e+00    3.50  6.00e+03
!iBuOH+CH3=CH4+C4H9Oi1  0.357e+00   3.65   7153.44
!iBuOH+CH3=CH4+C4H9Oi2  1.904e+00   3.46   4591.3
!! Updated by MRH 10/JUN/2010 (cbs-qb3 calculations w/1D hindered rotor
corrections)
iBuOH+CH3=CH4+C4H9Oi1   1.357e+00   3.65   7153.44
iBuOH+CH3=CH4+C4H9Oi2   1.904e+00   3.46   4591.3
!iBuOH+CH3=CH4+C4H9Oi4  2.32e+00    3.49  6.09e+03

iBuOH+CH2OH=C4H9Oi1+CH3OH     1.040E+06   1.800 15050.00
      !H_Abstraction estimate: (Average:) C/H3/Cs     C_rad/H2/O
iBuOH+CH2OH=C4H9Oi2+CH3OH     0.99140E+06 1.753 12532.12
      !H_Abstraction estimate: (Average:) C/H2/NonDeC     C_rad/H2/O
iBuOH+CH2OH=C4H9Oi3+CH3OH     0.99040E+06 1.786 13448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/O
iBuOH+CH2OH=C4H9Oi4+CH3OH     0.250E-04   5.000 12580.00
      !H_Abstraction estimate: (Average:) O/H/NonDeC     C_rad/H2/O

iBuOH+CH3O=C4H9Oi1+CH3OH      2.820E+11   0.000 7000.00
      !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
iBuOH+CH3O=C4H9Oi2+CH3OH      2.200E+11   0.000 4570.00
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeC
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iBuOH+CH3O=C4H9Oi3+CH3OH      3.173E9     0.95  5644.0
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_rad/NonDeC
C4H9Oi4+CH3OH=iBuOH+CH3O      2.820E+11   0.000 7000.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeC

!iBuOH+C2H5=C4H9Oi1+C2H6      2.040E+05   1.900 11050.00
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
!iBuOH+C2H5=C2H6+C4H9Oi1      2.20e-01    3.87  10.67e+03   !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C2H6+C4H9Oi1=iBuOH+C2H5       1.926e-05   5.28  7.78e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!iBuOH+C2H5=C4H9Oi2+C2H6      0.2100E+06  1.670 8530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
iBuOH+C2H5=C2H6+C4H9Oi2       1.41e-05    4.83  4.37e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!iBuOH+C2H5=C4H9Oi3+C2H6      2.040E+05   1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
iBuOH+C2H5=C2H6+C4H9Oi3       8.50e-06    5.01  5.01e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!C4H9Oi4+C2H6=iBuOH+C2H5      2.844e+12   0.0   9000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs
!C2H6+C4H9Oi4=iBuOH+C2H5            3.04e-02    4.52  2.34e+03    !MRH
CBS-QB3 RRHO calculation w/asymmetric Eckart
iBuOH+C2H5=C2H6+C4H9Oi4   1.43e-03   4.21   5.69e+03
iBuOH+CH3=CH4+C4H9Oi4   1.44e+01   3.1   6935.9
iBuOH+iC4H7=iC4H8+C4H9Oi4   1.62e-01   3.26   17.40e+03

iBuOH+C3H7-1=C4H9Oi1+C3H8     2.640E+05   1.900 12050.00
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
iBuOH+C3H7-1=C4H9Oi2+C3H8     5.040E+05   1.770 10530.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
iBuOH+C3H7-1=C4H9Oi3+C3H8     5.040E+05   1.770 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
iBuOH+C3H7-1=C4H9Oi4+C3H8     7.550E-05   4.000 5580.00
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H9Oi1+nC4H10=iBuOH+C4H9-1   1259.0            2.61  12920.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cs
iBuOH+C4H9-1=C4H9Oi2+nC4H10   3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
iBuOH+C4H9-1=C4H9Oi3+nC4H10   3.04E+06    1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9Oi4+nC4H10=iBuOH+C4H9-1   4.74E11     0.0   7000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H9Oi1+nC4H10=iBuOH+C4H9-2   3040.0      2.66  12100.0
      !H_Abstraction exact:   C_rad/H2/Cs     C/H2/NonDeC
C4H9Oi2+nC4H10=iBuOH+C4H9-2   15.2        3.19  10310.0
      !H_Abstraction exact:   C_rad/H/NonDeC     C/H2/NonDeC
iBuOH+C4H9-2=C4H9Oi3+nC4H10   3.04E06     1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H/NonDeC
C4H9Oi4+nC4H10=iBuOH+C4H9-2   7.25E10     0.0   4570.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H2/NonDeC


iBuOH+C2H5O-1=C4H9Oi1+C2H5OH  2077.0      2.71  13920.0
      !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
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iBuOH+C2H5O-1=C4H9Oi2+C2H5OH  3080.0      2.66  10100.0
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
iBuOH+C2H5O-1=C4H9Oi3+C2H5OH  3.04E+06    1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H9Oi4+C2H5OH=iBuOH+C2H5O-1  4.74E11     0.0   7000.0
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H7-14+iBuOH=C4H8-1+C4H9Oi1  6.080E+03   2.660 10100.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C4H7-14+iBuOH=C4H8-1+C4H9Oi2  3.080E+03   2.660 10100.00
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C4H7-14+iBuOH=C4H8-1+C4H9Oi3  3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H2/Cs
C4H8-1+C4H9Oi4=C4H7-14+iBuOH  1.420E+12   0.000 7000.00
      !H_Abstraction exact:   O_rad/NonDeC     C/H3/Cs

C4H8-1+C4H9Oi1=C4H7-24+iBuOH  2.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H8-1+C4H9Oi2=C4H7-24+iBuOH  1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H8-1+C4H9Oi3=C4H7-24+iBuOH  1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H2/OneDeC
C4H8-1+C4H9Oi4=C4H7-24+iBuOH  1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/OneDeC

C4H6-1+C4H9Oi1=C4H5-113+iBuOH 6.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H2/OneDeC
C4H6-1+C4H9Oi2=C4H5-113+iBuOH 3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C4H6-1+C4H9Oi3=C4H5-113+iBuOH 3.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H2/OneDeC
C4H6-1+C4H9Oi4=C4H5-113+iBuOH 1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/OneDeC

!C3H6+C4H9Oi1=aC3H5+iBuOH     2.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C3H6+C4H9Oi1=iBuOH+aC3H5      1.01e-04    4.75  4.13e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!C3H6+C4H9Oi2=aC3H5+iBuOH     1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/NonDeC     C/H2/OneDeC
C3H6+C4H9Oi2=iBuOH+aC3H5      4.92e-06    4.98  3.18e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!C3H6+C4H9Oi3=aC3H5+iBuOH     1.040E+06   1.886 9448.33
      !H_Abstraction estimate: (Average:) C_rad/H/CsO     C/H2/OneDeC
C3H6+C4H9Oi3=iBuOH+aC3H5      9.33e-06    4.97  3.64e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!C3H6+C4H9Oi4=aC3H5+iBuOH     1.680E+09   1.000 5105.00
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H2/OneDeC
C3H6+C4H9Oi4=iBuOH+aC3H5      3.57e-01    3.90  1.81e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart

iBuOH+O2=C4H9Oi1+HO2    1.206E14    0.0   51.87e+03   !H_Abstraction
exact:      C/H3/Cs     O2b
iBuOH+O2=C4H9Oi2+HO2    1.588E14    0.0   47.69e+03   !H_Abstraction
exact:      C/H2/NonDeC     O2b
iBuOH+O2=C4H9Oi3+HO2    1.588E14    0.0   47.69e+03   !H_Abstraction
estimate: (Average:)    C/H2/CsO     O2b
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iBuOH+O2=C4H9Oi4+HO2    2.325E12    0.0   74.12e+03   !H_Abstraction
estimate: (Average:)    O/H/NonDeC     O2b

iBuOH+O=C4H9Oi1+OH      9.540E+04   2.710 2106.00     !H_Abstraction
exact:      C/H3/Cs     O_atom_triplet
!iBuOH+O=C4H9Oi2+OH     4.289E+05   2.65  2583.65     !H_Abstraction
exact:      C/H2/NonDeC     O_atom_triplet
!The following comes from: W. Tsang, "Chemical kinetic database for
comubstion chemistry.  Part IV.  Isobutane"
!     J. Phys. Chem. Ref. Data. 19 (1990) 1-68
!The kinetic rate is for iso-butane + O = OH + tert-C4H9
!iBuOH+O=C4H9Oi2+OH     1.57E+05    2.5         1113.77
iBuOH+O=C4H9Oi2+OH      0.78E+05    2.5         1113.77
iBuOH+O=C4H9Oi3+OH      1.289E+05   2.79  2183.65     !H_Abstraction
estimate: (Average:)    C/H2/CsO     O_atom_triplet
iBuOH+O=C4H9Oi4+OH      1.000E+13   0.000 4690.00     !H_Abstraction
exact:      O/H/NonDeC     O_atom_triplet

!MRH 7/JUN/2010

!CBS-QB3 calculations (w/o HR corrections)
H2O2+C4H9Oi1=iBuOH+HO2  3.01e+00    3.28  1.05e+03
H2O2+C4H9Oi2=iBuOH+HO2  2.91e+00    3.31  1.41e+03
H2O2+C4H9Oi3=iBuOH+HO2  5.69e+01    3.04  1.21e+03
H2O2+C4H9Oi4=iBuOH+HO2  34.6        3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    O_rad/NonDeC     H2O2

!iBuOH+O2 via reverse of disproportionation
!HO2+C4H9Oi4=O2+iBuOH   1.7499999999999977E10   0.0   -3.275e+03
      !Disproportionation estimate: (Average:)  O_Orad     O_rad/NonDeC
!HO2+C4H9Oi3=O2+iBuOH   2.9999999999999976E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H/CsO
!HO2+C4H9Oi2=O2+iBuOH   2.9999999999999976E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/Cs3
!HO2+C4H9Oi1=O2+iBuOH   2.9999999999999976E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/Cs

!O2 + radical = ketone/enol + HO2
O2+C4H9Oi3=HO2+C4H8O-i3 4.6826e+11 0.3321 -1.0635e+03 !from Zador et al
calculated for CH3CHOH+O2=HO2+CH3CHO (consistant with RMG) edited by MHS
04.27.11
!O2+C4H9Oi3=HO2+C4H8O-i3            1.14418E13  0.0   0.0e+03
      !Disproportionation_O2d exact:      O2d     O_Csrad
O2+C4H9Oi3=HO2+C4H8O-i2       2.4088E10   0.0   0.0e+03
      !Disproportionation_O2d exact:      O2d     C/H/NdNd_Csrad

!C3H6O-enol chemistry
C3H6O-enol+H=C3H5O-enol2+H2   129900.0    2.38  5.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad
C3H6O-enol+OH=C3H5O-enol2+H2O 1.9909776464507412E6    1.75
      3.7893749999999997e+03  !H_Abstraction estimate: (Average:)
      C/H3/Cd     O_pri_rad
C3H5O-enol2+H2O2=C3H6O-enol+HO2     2.0304986547865194
      3.2899999999999996      1.0725e+03  !H_Abstraction estimate:
(Average:)  C_rad/H2/Cd     H2O2
C3H6O-enol+O=C3H5O-enol2+OH   2850.0000000000005      3.05  3.123e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_atom_triplet
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C3H6O-enol+CH3=C3H5O-enol2+CH4      241.20000000000002      2.92
      7.16e+03    !H_Abstraction exact:   C/H3/Cd     C_methyl
!CH3+C2H3O-1=C3H6O-enol 7.23E13     0.0   0.0e+03     !R_Recombination
exact:      Cd_pri_rad     C_methyl

C3H6O-enol+H=C3H5OJ(12)+H2    1.3E11      0.82  7.75e+03
      !H_Abstraction exact:   O/H/OneDe     H_rad
C3H6O-enol+OH=C3H5OJ(12)+H2O  17.3  3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    O/H/OneDe     O_pri_rad
C3H6O-enol+O=C3H5OJ(12)+OH    1.0000000000000002E13   0.0   4.69e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_atom_triplet
C3H6O-enol+CH3=C3H5OJ(12)+CH4 90700.0     2.04  10.85e+03
      !H_Abstraction exact:   O/H/OneDe     C_methyl
C3H5OJ(12)+H2O2=C3H6O-enol+HO2 6.99e-02 3.75 10.89e+03  !MHS 04/27/11
(CBS-QB3 with 1DHR for C4H7OJ(12)+H2O2=C4H8O-enol+HO2)
!C3H5OJ(12)+H2O2=C3H6O-enol+HO2     34.6  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/OneDe     H2O2

!C3H6O-enol2 chemistry
C3H6O-enol2+H=C3H5O-enol2+H2  139799.9999999995 2.36  5.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     H_rad
C3H6O-enol2+OH=C3H5O-enol2+H2O      2.6681027652763863E9    0.95
      5.644e+03   !H_Abstraction estimate: (Average:) C/H2/OneDeO
O_pri_rad
C3H6O-enol2+HO2=C3H5O-enol2+H2O2    2.6681027652763863E9    0.95
      5.644e+03   !H_Abstraction estimate: (Average:) C/H2/OneDeO
O_rad/NonDeO
C3H6O-enol2+O=C3H5O-enol2+OH  47800.00000000004 2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O_atom_triplet
C3H6O-enol2+CH3=C3H5O-enol2+CH4     1.460000000000003E13    0.0
      14.4e+03    !H_Abstraction estimate: (Average:) C/H2/OneDeO
C_methyl

!C3H5O-enol chemistry
!O2+C3H5O-enol2=HO2+C3H4O     1.14418E13  0.0   0.0e+03
      !Disproportionation_O2d exact:      O2d     O_Csrad
O2+C3H5O-enol2=HO2+C3H4O      4.6826e+11 0.3321 -1.0635e+03 !from rate
calculated by Zador et al for CH3CHOH+O2=HO2+CH3CHO (consistent with
RMG) edited by MRH 05.12.11

!C3H7O-N2 chemistry
!replaced w/pdep rate coefficients
!C3H6O-enol2+H=C3H7O-N2 2.01E13     0.0   2.1e+03
      !R_Addition_MultipleBond exact:     Cd/H2_Cd/H/Nd     H_rad
!C3H6+OH=C3H7O-N2 2.7099999999999966E12   0.0   0.0e+03
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H2_Cd/H/Nd
O_pri_rad
!C3H6O-enol+H=C3H7O-N2  1.0000000000000002E13   0.0   2.9e+03
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/H/Nd
H_rad

!C4H8O-i1, C4H8O-i2, and C4H8O-i3 chemistry
!OH+iC4H7=C4H8O-i1      1.4157153560053182E13   -0.15
      0.2916666666666667e+03  !R_Recombination estimate: (Average:)
      O_pri_rad     C_rad/H2/Cd
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!CH2OH+sC3H5=C4H8O-i1   1.4157153560053182E13   -0.15
      0.2916666666666667e+03  !R_Recombination estimate: (Average:)
      C_rad/H2/O     Cd_rad/NonDe
!OH+HCC[CH3]2=C4H8O-i2  1.4157153560053182E13   -0.15
      0.2916666666666667e+03  !R_Recombination estimate: (Average:)
      O_pri_rad     Cd_pri_rad
!HCO+C3H7-2=C4H8O-i3    1.4157153560053182E13   -0.15
      0.2916666666666667e+03  !R_Recombination estimate: (Average:)
      CO_pri_rad     C_rad/H/NonDeC
!C3H5OJ(12)+CH3=C4H8O-i3      6.800000000000021E14    -0.68 0.0e+03
      !R_Recombination estimate: (Average:)     C_rad/H/OneDeC
C_methyl

! 9/JUN/2010
!replaced third-body rate constant from Marinov w/RMG estimate
!CH3CHO+H=C2H5O-2 7.299E11    0.17975     2.98508e+03
      !R_Addition_MultipleBond estimate: (Average:)   OCO     H_rad

!acetone oxidation chemistry
acetone+O=CH2C[O]CH3+OH 5700.0      3.05  3.123e+03   !H_Abstraction
estimate: (Average:)    C/H3/CO     O_atom_triplet
CH2C[O]CH3+H2O2=acetone+HO2   2.0305      3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/CO     H2O2
HO2+CH2C[O]CH3=O2+acetone     3.0E11      0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O_Orad     C_rad/H2/CO
!C2H6+CO=acetone  6456.0      3.29  104.5e+03   !1,2_Insertion exact:
      CO_birad     C_methyl_C_methyl

! 10/JUN/2010
! Following rate from: W. Tsang; "Chemical kinetic database for
combustion chemistry.  Part V.  Propene,"
! J. Phys. Chem. Ref. Data 20 (1991) 221-273
! The rate is for the reaction CH2O+aC3H5=HCO+C3H6
!CH2O+iC4H7=HCO+iC4H8   1.26e+08    1.9   18183.56
CH2O+iC4H7=HCO+iC4H8    6.13e-02    3.95  12.22e+03   !CBS-QB3
calculation, w/o HR correction, w/ asymmetric Eckart tunneling

!H-abstraction of C4H8O-enol to CH3CH2CHCHO*
C4H8O-enol+CH3=C4H7OJ(12)+CH4 90700.0     2.04  10.85e+03
      !H_Abstraction exact:   O/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -16.98723247841039 kcal/mol

C4H8O-enol+H=C4H7OJ(12)+H2    1.3E11      0.82  7.75e+03
      !H_Abstraction exact:   O/H/OneDe     H_rad
      deltaHrxn(T=298K) = -16.196029540350953 kcal/mol

C4H8O-enol+OH=C4H7OJ(12)+H2O  17.3  3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    O/H/OneDe     O_pri_rad       deltaHrxn(T=298K)
= -30.799657804705106 kcal/mol

C4H8O-enol+O=C4H7OJ(12)+OH    1.0000000000000002E13   0.0   4.69e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -14.735671136505083 kcal/mol

!C4H8O-enol+O2=C4H7OJ(12)+HO2 651492.4520475856 2.1197348484848484
      16.23166856060606e+03   !H_Abstraction estimate: (Average:)
```

```
      O/H/OneDe     O2b       deltaHrxn(T=298K) = 38.89549762574563
kcal/mol
!C4H8O-enol+O2=C4H7OJ(12)+HO2 651492.45   2.12  26.23167856060606e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 38.89549762574563 kcal/mol
C4H8O-enol+O2=C4H7OJ(12)+HO2  1.0E11      0.0   38.28614e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 38.28613942203209 kcal/mol

C4H7OJ(12)+H2O2=C4H8O-enol+HO2 6.99e-02 3.75 10.89e+03  !MHS 04/20/11
!C4H7OJ(12)+H2O2=C4H8O-enol+HO2     34.6  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/OneDe     H2O2
      deltaHrxn(T=298K) = -0.4273637640552508 kcal/mol

!H-abstraction of CH3CHCHCHO
CH3CCHCHO+CH4=CH3CHCHCHO+CH3  6.359999999999994E14    0.0   13.7e+03
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C_methane
      deltaHrxn(T=298K) = -4.010510488403334 kcal/mol
CH3CHCHCHO+CH3=CH3CHCHCO+CH4  1.0533755265810958E8    1.145 6.325e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -21.986868671912923 kcal/mol
CH3CCHCHO+H2=CH3CHCHCHO+H     6.02E12     0.0   10.6e+03
      !H_Abstraction exact:   H2     Cd_rad/NonDeC
      deltaHrxn(T=298K) = -4.801713426462768 kcal/mol
CH3CHCHCHO+H=CH3CHCHCO+H2     4.0000000000000016E13   0.0   4.21e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     H_rad
      deltaHrxn(T=298K) = -21.195665733853488 kcal/mol
CH3CHCHCHO+OH=CH3CCHCHO+H2O   1110000.0   2.0   1.45e+03
      !H_Abstraction exact:   Cd/H/NonDeC     O_pri_rad
      deltaHrxn(T=298K) = -9.801914837891381 kcal/mol
!CH3CHCHCHO+OH=CH3CHCHCO+H2O  5.486346689738067E12    0.0   5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -35.799293998207645 kcal/mol
CH3CHCHCHO+OH=CH3CHCHCO+H2O         1.00E13     0.0   0.0   !Estimate,
based on CH3CHO+OH=H2O+CH3CO
CH3CHCHCHO+O=CH3CCHCHO+OH     6.02E10     0.7   7.63e+03
      !H_Abstraction exact:   Cd/H/NonDeC     O_atom_triplet
      deltaHrxn(T=298K) = 6.2620718303086385 kcal/mol
CH3CHCHCHO+O=CH3CHCHCO+OH     4.999999999999991E12    0.0   1.79e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -19.73530733000762 kcal/mol
CH3CHCHCHO+O2=CH3CCHCHO+HO2   3.4289569352522535E9    1.1959166666666667
      55.218083333333329e+03  !H_Abstraction estimate: (Average:)
      Cd/H/NonDeC     O2b           deltaHrxn(T=298K) =
59.893240592559344 kcal/mol
!CH3CHCHCHO+O2=CH3CHCHCO+HO2  1.2039999999999992E14   0.0   39.15e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O2b
      deltaHrxn(T=298K) = 33.89586143224309 kcal/mol
!CH3CHCHCHO+O2=CH3CHCHCO+HO2 3.00E+13  0.0  36000.0   ! ESTIMATE, based
on C3H4O+O2=HO2+C3H3O-enone
CH3CCHCHO+H2O2=CH3CHCHCHO+HO2 28.799999999999997      3.1   6.94e+03
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     H2O2
      deltaHrxn(T=298K) = -21.42510673086897 kcal/mol
CH3CHCHCHO+HO2=CH3CHCHCO+H2O2 5.486346689738067E12    0.0   5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_rad/NonDeO
      deltaHrxn(T=298K) = -4.572272429447285 kcal/mol
```

```
!beta-scission of C4H5O radicals
pC3H4+HCO=CH3CCHCHO     5.2E11      0.0   6.56e+03
      !R_Addition_MultipleBond estimate: (Average:)   Ct/H_Ct/Nd
CO_pri_rad        deltaHrxn(T=298K) = -25.60323968466651 kcal/mol
!pC3H5+CO=CH3CHCHCO     1.51E11     0.0   4.81e+03    !R_Addition_COm
exact:      COm     Cd_pri_rad      deltaHrxn(T=298K) = -
34.620991396552014 kcal/mol

!H-Abstraction of C4H8O-enol2 and C4H8O-enol3 by O/O2/HO2
C4H8O-enol2+O=C4H7O-13+OH     2850.0      3.05  3.123e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -15.365533040947678 kcal/mol
C4H8O-enol2+O=C4H7O_1_2+OH    47800.0     2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O_atom_triplet
      deltaHrxn(T=298K) = -21.69492404386383 kcal/mol
C4H8O-enol3+O=C4H7O-13+OH     47800.0     2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_atom_triplet
      deltaHrxn(T=298K) = -17.13537016711224 kcal/mol

C4H8O-enol2+O2=C4H7O-13+HO2   1.206E14    0.0   51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 38.26563572130303 kcal/mol
C4H8O-enol2+O2=C4H7O_1_2+HO2  1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O2b
      deltaHrxn(T=298K) = 31.93624471838688 kcal/mol
C4H8O-enol3+O2=C4H7O-13+HO2   1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O2b
      deltaHrxn(T=298K) = 36.49579859513847 kcal/mol

!C4H7O-13+H2O2=C4H8O-enol2+HO2      2.0305      3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     H2O2
      deltaHrxn(T=298K) = 0.20249814038734826 kcal/mol
C4H8O-enol2+HO2=C4H7O-13+H2O2 2.668E9     0.95  5.644e+03   !Estimate,
based on C4H8O-enol2+HO2=C4H7O_1_2+H2O2
C4H8O-enol2+HO2=C4H7O_1_2+H2O2      2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O_rad/NonDeO
      deltaHrxn(T=298K) = -6.531889143303495 kcal/mol
C4H8O-enol3+HO2=C4H7O-13+H2O2 2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_rad/NonDeO
      deltaHrxn(T=298K) = -1.9723352665519052 kcal/mol

!H-Abstraction of C4H8O-enol3, C4H8O-enol, and C3H4O-enone
C4H8O-enol3+H=C4H7O-14+H2     1727370.8   2.3   1.330e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     H_rad
      deltaHrxn(T=298K) = -8.8070460603099 kcal/mol
C4H8O-enol3+CH3=C4H7O-14+CH4  3039788.2   1.886 9.448e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_methyl
      deltaHrxn(T=298K) = -9.598248998369336 kcal/mol
C3H4O-enone+CH3=C3H3O-enone+CH4     241.2 2.92  7.16e+03
      !H_Abstraction exact:   C/H3/Cd     C_methyl
      deltaHrxn(T=298K) = -27.279411197971093 kcal/mol
C4H8O-enol3+OH=C4H7O-14+H2O   2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_pri_rad
      deltaHrxn(T=298K) = -23.41067432466405 kcal/mol
C4H8O-enol3+O=C4H7O-14+OH     47800.0     2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_atom_triplet
      deltaHrxn(T=298K) = -7.346687656464031 kcal/mol
```

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C4H8O-enol+O=C4H7O_1_2+OH     47800.0     2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_atom_triplet
      deltaHrxn(T=298K) = -17.135370150143657 kcal/mol
C4H8O-enol3+O2=C4H7O-14+HO2   1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O2b
      deltaHrxn(T=298K) = 46.28448110578668 kcal/mol
C4H8O-enol+O2=C4H7O_1_2+HO2   1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O2b
      deltaHrxn(T=298K) = 36.49579861210705 kcal/mol
C3H4O-enone+O2=C3H3O-enone+HO2      1.206E14    0.0   51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 28.603318906184917 kcal/mol
C4H7O-14+H2O2=C4H8O-enol3+HO2 2.97  3.39  1.4e+03     !H_Abstraction
exact:      H2O2     C_rad/H/CsO          deltaHrxn(T=298K) = -
7.816347244096299 kcal/mol
C4H8O-enol+HO2=C4H7O_1_2+H2O2 2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeC     O_rad/NonDeO
      deltaHrxn(T=298K) = -1.972335249583324 kcal/mol
!C3H4O-enone+HO2=C3H3O-enone+H2O2   1.991E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_rad/NonDeO
      deltaHrxn(T=298K) = -9.864814955505459 kcal/mol
C3H3O-enone+H2O2=C3H4O-enone+HO2    2.0305      3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     H2O2
      deltaHrxn(T=298K) = -2.7196315623268745 kcal/mol

!C2H3+C2H4O=C4H7O-14    149.03      3.0074      10.1708e+03
      !R_Addition_MultipleBond estimate: (Average:)   Cd_pri_rad
Cd/H2_Cd/H/Nd           deltaHrxn(T=298K) = -34.63691045890636 kcal/mol

!C5H5+C5H5=biC5H5 2e+13 0.0   0.0   !Assumed R_recombination rate
!PDepNetwork biC5H5
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     biC5H5      65.33 55.19 41.26 52.63 62.31 69.9  80.85 88.47 99.89
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C5H5        63.08 71.78 18.65 24.13 28.95 32.88 38.15 41.95 47.42
!Burcat 07-Jan-2011
!     C5H4C5H5    89.3  57.66 37.72 49.93 59.8  67.39 78.26 85.64 97.18
      null
!Here are the path reactions and their high-P limit kinetics:
!     C5H5+C5H5=biC5H5  2.000e+13    0.00        0.00
!     C5H4C5H5+H=biC5H5       5.0000000e+13      0.00000
0.0000000e+00

C5H5+C5H5(+m)=biC5H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (biC5H5) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -60.82448510452576 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4871000e+00 1.4412000e+00 -1.1395000e-01 /
CHEB / -5.4836000e+00 6.0006000e-01 1.5109000e-01 /
CHEB / -1.9084000e+00 5.0848000e-02 -3.1527000e-02 /
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CHEB / -3.3694000e-01 -6.9428000e-02 -9.1145000e-03 /
CHEB / 1.3184000e-01 -2.2111000e-02 3.9821000e-03 /

!C5H4C5H5+H(+m)=biC5H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (biC5H5) High-P Limit: R_Recombination estimate:
(Average:) C_rad/Cs     H_rad       deltaHrxn(T=298K) = -
76.06220193304544 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 5.9014000e+00 1.9999000e+00 -4.6598000e-05 /
!CHEB / -3.5414000e+00 9.0061000e-05 6.2682000e-05 /
!CHEB / -1.0971000e+00 -1.3440000e-05 -9.3566000e-06 /
!CHEB / -1.7508000e-01 -1.9841000e-05 -1.3807000e-05 /
!CHEB / 1.0015000e-01 1.0848000e-05 7.5502000e-06 /

C5H4C5H5+H(+m)=C5H5+C5H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (biC5H5) deltaHrxn(T=298K) = -15.237716828519687 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3853000e+01 -1.4906000e-05 -1.0374000e-05 /
CHEB / -1.2623000e-01 2.4281000e-05 1.6899000e-05 /
CHEB / 9.4453000e-04 -1.2678000e-05 -8.8239000e-06 /
CHEB / 2.4004000e-04 3.6834000e-06 2.5637000e-06 /
CHEB / 1.2646000e-03 -3.2608000e-07 -2.2708000e-07 /

! Following four rate coefficient expressions from:
! A.M. Mebel, V.V. Kislov
! "Can the C5H5+C5H5=>C10H10=>C10H9+H/C10H8+H2 reaction produce
naphthalene?
!     An ab initio / RRKM study"
! J. Phys. Chem. A 113 (2009) 9825-9833
biC5H5=H+C5H4C5H5 1.97e+16    -0.21 78265.0
biC5H5=H+C10H9          8.86e+12    -0.09 69961.0
C5H4C5H5=H+fulvalene    5.64e+19    -1.24 59295.0
C5H4C5H5=H+C10H8        4.53e+05    1.83  36345.0

! J. Aguilera-Iparraguirre, W. Klopper
! "DFT study of the formation of napthalene and phenanthrene from
reactions of
!     phenyl with vinyl- and phenylacetylene"
! J. Chem. Theory Comput. 3 (2007) 139-145
C10H9=H+C10H8     7.843e+07   0.97  34894.84

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! 21Jul2010: Iso-butanol chemistry !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

C4H8O-i1+H=iC4H7OJ(15)+H2     1398000     2.36  1.11e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     H_rad
      deltaHrxn(T=298K) = -23.66539390515253 kcal/mol
C4H8O-i1+H=C4H7OJ(79)+H2      8.7E8 1.39  10.07e+03   !H_Abstraction
exact:      O/H/NonDeC     H_rad          deltaHrxn(T=298K) = -
0.13767450866680248 kcal/mol
C4H8O-i1+H=iC4H7OJ(17)+H2     1299000     2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad       deltaHrxn(T=298K)
= -15.996100012948432 kcal/mol
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C4H8O-i2+H=iC4H7OJ(15)+H2     2598000     2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad       deltaHrxn(T=298K)
= -15.996099953245032 kcal/mol
C4H8O-i2+H=iC4H7OJ(30)+H2     1.3E11      0.82  7.75e+03
      !H_Abstraction exact:   O/H/OneDe     H_rad
      deltaHrxn(T=298K) = -16.19602954025756 kcal/mol
C4H8O-i3+H=iC4H7OJ(48)+H2     3.768E8     1.75  7.51e+03
      !H_Abstraction exact:   C/H3/Cs     H_rad       deltaHrxn(T=298K)
= -3.0974230222921193 kcal/mol
!C4H8O-i3+H=iC4H7OJ(30)+H2    3020000     2.16  -0.45e+03
      !H_Abstraction exact:   C/H/Cs2     H_rad       deltaHrxn(T=298K)
= -10.926762447943206 kcal/mol
C4H8O-i3+H=iC4H7OJ(30)+H2     1.04e+07    1.84  3.03e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C4H8O-i3+H=iC4H7OJ(51)+H2     6.40E8      1.76  0.67e+03
      !H_Abstraction exact:   CO/H/NonDe     H_rad
      deltaHrxn(T=298K) = -15.196186361773613 kcal/mol

C4H8O-i1+CH3=iC4H7OJ(15)+CH4  5.46E13     0.0         10.4e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     C_methyl
      deltaHrxn(T=298K) = -24.456596843211965 kcal/mol
C4H7OJ(79)+CH4=C4H8O-i1+CH3   6.2E-4      5.0         5.58e+03
      !H_Abstraction exact:   C_methane     O_rad/NonDeC
      deltaHrxn(T=298K) = 0.9288774467262364 kcal/mol
C4H8O-i1+CH3=iC4H7OJ(17)+CH4  241.2 2.92  7.16e+03    !H_Abstraction
exact:      C/H3/Cd     C_methyl          deltaHrxn(T=298K) = -
16.787302951007867 kcal/mol
C4H8O-i2+CH3=iC4H7OJ(15)+CH4  482.4 2.92  7.16e+03    !H_Abstraction
exact:      C/H3/Cd     C_methyl          deltaHrxn(T=298K) = -
16.787302891304467 kcal/mol
C4H8O-i2+CH3=iC4H7OJ(30)+CH4  90700.0     2.04  10.85e+03
      !H_Abstraction exact:   O/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -16.98723247831699 kcal/mol
C4H8O-i3+CH3=iC4H7OJ(48)+CH4  1668000     1.9         11.05e+03
      !H_Abstraction exact:   C/H3/Cs     C_methyl
      deltaHrxn(T=298K) = -3.888625960351554 kcal/mol
C4H8O-i3+CH3=iC4H7OJ(30)+CH4  2.73E13     0.0         8.9e+03
      !H_Abstraction exact:   C/H/Cs2     C_methyl
      deltaHrxn(T=298K) = -11.717965386002641 kcal/mol
C4H8O-i3+CH3=iC4H7OJ(51)+CH4  29200.0     2.29  5.44e+03
      !H_Abstraction exact:   CO/H/NonDe     C_methyl
      deltaHrxn(T=298K) = -15.987389299833048 kcal/mol

C4H8O-i1+CH2OH=iC4H7OJ(15)+CH3OH    3039788           1.886 9.448e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     C_rad/H2/O
      deltaHrxn(T=298K) = -15.530481083276783 kcal/mol
C4H7OJ(79)+CH3OH=C4H8O-i1+CH2OH     1.991E7           1.75  3.789e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     C/H3/O
      deltaHrxn(T=298K) = -7.997238313208946 kcal/mol
C4H8O-i1+CH2OH=iC4H7OJ(17)+CH3OH    8.7173E12   0.0         17.333e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     C_rad/H2/O
      deltaHrxn(T=298K) = -7.861187191072688 kcal/mol
C4H8O-i2+CH2OH=iC4H7OJ(15)+CH3OH    1.7435E13   0.0         17.333e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     C_rad/H2/O
      deltaHrxn(T=298K) = -7.8611871313692845 kcal/mol
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C4H8O-i2+CH2OH=iC4H7OJ(30)+CH3OH    136.06            2.70  6.460e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/O
      deltaHrxn(T=298K) = -8.061116718381811 kcal/mol
iC4H7OJ(48)+CH3OH=C4H8O-i3+CH2OH    9407453           1.75  12.532e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cs     C/H3/O
      deltaHrxn(T=298K) = -5.037489799583632 kcal/mol
C4H8O-i3+CH2OH=iC4H7OJ(30)+CH3OH    1.6208E9    1.00  11.129e+03
      !H_Abstraction estimate: (Average:) C/H/Cs2     C_rad/H2/O
      deltaHrxn(T=298K) = -2.79184962606746 kcal/mol
C4H8O-i3+CH2OH=iC4H7OJ(51)+CH3OH    3.8000E11   0.0         7.21e+03
      !H_Abstraction estimate: (Average:) CO/H/NonDe     C_rad/H2/O
      deltaHrxn(T=298K) = -7.0612735398978685 kcal/mol

C4H8O-i1+O=iC4H7OJ(15)+OH     47800 2.71  2.11e+03    !H_Abstraction
estimate: (Average:)    C/H2/OneDeO     O_atom_triplet
      deltaHrxn(T=298K) = -22.20503550130666 kcal/mol
C4H8O-i1+O=C4H7OJ(79)+OH      1.0E13      0.0         4.69e+03
      !H_Abstraction exact:   O/H/NonDeC     O_atom_triplet
      deltaHrxn(T=298K) = 1.3226838951790683 kcal/mol
C4H8O-i1+O=iC4H7OJ(17)+OH     2850  3.05  3.123e+03   !H_Abstraction
estimate: (Average:)    C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -14.535741609102562 kcal/mol
C4H8O-i2+O=iC4H7OJ(15)+OH     5700  3.05  3.123e+03   !H_Abstraction
estimate: (Average:)    C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -14.535741549399162 kcal/mol
C4H8O-i2+O=iC4H7OJ(30)+OH     1.0E13      0.0         4.69e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -14.735671136411689 kcal/mol
C4H8O-i3+O=iC4H7OJ(48)+OH     5700.0      3.05  3.123e+03
      !H_Abstraction exact:   C/H3/Cs     O_atom_triplet
      deltaHrxn(T=298K) = -1.6370646184462494 kcal/mol
C4H8O-i3+O=iC4H7OJ(30)+OH     157000      2.5         1.11e+03
      !H_Abstraction estimate: (Average:) C/H/Cs2     O_atom_triplet
      deltaHrxn(T=298K) = -9.466404044097338 kcal/mol
C4H8O-i3+O=iC4H7OJ(51)+OH     5.0E12      0.0         1.79e+03
      !H_Abstraction exact:   CO/H/NonDe     O_atom_triplet
      deltaHrxn(T=298K) = -13.735827957927743 kcal/mol

C4H8O-i1+OH=iC4H7OJ(15)+H2O   2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O_pri_rad
      deltaHrxn(T=298K) = -38.269022169506684 kcal/mol
C4H8O-i1+OH=C4H7OJ(79)+H2O    17.3  3.4         -1.14e+03
      !H_Abstraction exact:   O/H/NonDeC     O_pri_rad
      deltaHrxn(T=298K) = -14.741302773020955 kcal/mol
C4H8O-i1+OH=iC4H7OJ(17)+H2O   1.991E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
      deltaHrxn(T=298K) = -30.599728277302585 kcal/mol
C4H8O-i2+OH=iC4H7OJ(15)+H2O   3.982E7     1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
      deltaHrxn(T=298K) = -30.599728217599186 kcal/mol
C4H8O-i2+OH=iC4H7OJ(30)+H2O   17.3  3.4         -1.14e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -30.799657804611712 kcal/mol
C4H8O-i3+OH=iC4H7OJ(48)+H2O   7200000     2.0         0.86e+03
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
      deltaHrxn(T=298K) = -17.70105128664627 kcal/mol
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C4H8O-i3+OH=iC4H7OJ(30)+H2O   6.561E8     0.95  3.99775e+03
      !H_Abstraction estimate: (Average:) C/H/Cs2     O_pri_rad
      deltaHrxn(T=298K) = -25.53039071229736 kcal/mol
C4H8O-i3+OH=iC4H7OJ(51)+H2O   1.0E13      0.0         0.0e+03
      !H_Abstraction exact:   CO/H/NonDe     O_pri_rad
      deltaHrxn(T=298K) = -29.799814626127766 kcal/mol

C4H8O-i1+O2=iC4H7OJ(15)+HO2   1.588E14    0.0         47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O2b
      deltaHrxn(T=298K) = 31.42613326094405 kcal/mol
C4H8O-i1+O2=C4H7OJ(79)+HO2    674422            2.106 54.95e+03
      !H_Abstraction estimate: (Average:) O/H/NonDeC     O2b
      deltaHrxn(T=298K) = 54.95385265742978 kcal/mol
C4H8O-i1+O2=iC4H7OJ(17)+HO2   1.206E14    0.0         51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 39.095427153148144 kcal/mol
C4H8O-i2+O2=iC4H7OJ(15)+HO2   2.412E14    0.0         51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 39.09542721285155 kcal/mol
!C4H8O-i2+O2=iC4H7OJ(30)+HO2  674422            2.106 16.163e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 38.89549762583902 kcal/mol
C4H8O-i2+O2=iC4H7OJ(30)+HO2   1.00E+11    0.0         38.286e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 38.28613942212549 kcal/mol
C4H8O-i3+O2=iC4H7OJ(48)+HO2   2.412E14    0.0         51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b         deltaHrxn(T=298K)
= 51.99410414380446 kcal/mol
C4H8O-i3+O2=iC4H7OJ(30)+HO2   1.588E14    0.0         43.92e+03
      !H_Abstraction estimate: (Average:) C/H/Cs2     O2b
      deltaHrxn(T=298K) = 44.16476471815337 kcal/mol
C4H8O-i3+O2=iC4H7OJ(51)+HO2   1.204E14    0.0         39.15e+03
      !H_Abstraction exact:   CO/H/NonDe     O2b      deltaHrxn(T=298K)
= 39.89534080432297 kcal/mol

C4H8O-i1+HO2=iC4H7OJ(15)+H2O2 2.668E9     0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O_rad/NonDeO
      deltaHrxn(T=298K) = -7.042000600746327 kcal/mol
C4H7OJ(79)+H2O2=C4H8O-i1+HO2  34.6  3.4         -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     H2O2
      deltaHrxn(T=298K) = -16.485718795739402 kcal/mol
iC4H7OJ(17)+H2O2=C4H8O-i1+HO2 2.0305      3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     H2O2
      deltaHrxn(T=298K) = -0.627293291457768 kcal/mol
iC4H7OJ(15)+H2O2=C4H8O-i2+HO2 2.0305      3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     H2O2
      deltaHrxn(T=298K) = -0.6272933511611711 kcal/mol
iC4H7OJ(30)+H2O2=C4H8O-i2+HO2 34.6  3.4         -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/OneDe     H2O2
      deltaHrxn(T=298K) = -0.4273637641486445 kcal/mol
iC4H7OJ(48)+H2O2=C4H8O-i3+HO2 2.0305      3.29  1.0725e+03
      !H_Abstraction exact:   H2O2     C_rad/H2/Cs
      deltaHrxn(T=298K) = -13.525970282114088 kcal/mol
iC4H7OJ(30)+H2O2=C4H8O-i3+HO2 34.6  3.05  1.02e+03
      !H_Abstraction estimate: (Average:) C_rad/Cs2     H2O2
      deltaHrxn(T=298K) = -5.6966308564629955 kcal/mol
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iC4H7OJ(51)+H2O2=C4H8O-i3+HO2 337211      2.11  16.163e+03
      !H_Abstraction estimate: (Average:) CO_rad/NonDe     H2O2
      deltaHrxn(T=298K) = -1.427206942632587 kcal/mol

C4H6Oi-13+H=iC4H5OJ(14)+H2    8.0700E7    1.76  0.67e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     H_rad
      deltaHrxn(T=298K) = -21.19566577493474 kcal/mol
C4H6Oi-13+H=iC4H5OJ(15)+H2    1299000.0   2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad       deltaHrxn(T=298K)
= -15.996100117827943 kcal/mol
C4H6Oi-12+H=iC4H5OJ(14)+H2    2598000.0   2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad       deltaHrxn(T=298K)
= -26.73127895714871 kcal/mol

C4H6Oi-13+CH3=iC4H5OJ(14)+CH4 1.0534E8    1.145 6.325e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -21.986868712994173 kcal/mol
C4H6Oi-13+CH3=iC4H5OJ(15)+CH4 241.2       2.92  7.16e+03
      !H_Abstraction exact:   C/H3/Cd     C_methyl
      deltaHrxn(T=298K) = -16.787303055887378 kcal/mol
C4H6Oi-12+CH3=iC4H5OJ(14)+CH4 482.4       2.92  7.16e+03
      !H_Abstraction exact:   C/H3/Cd     C_methyl
      deltaHrxn(T=298K) = -27.522481895208145 kcal/mol

C4H6Oi-13+CH2OH=iC4H5OJ(14)+CH3OH   1.0534E8    1.145 6.325e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     C_rad/H2/O
      deltaHrxn(T=298K) = -13.060752953058994 kcal/mol
C4H6Oi-13+CH2OH=iC4H5OJ(15)+CH3OH   8.7173E12   0.0         17.333e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     C_rad/H2/O
      deltaHrxn(T=298K) = -7.861187295952192 kcal/mol
C4H6Oi-12+CH2OH=iC4H5OJ(14)+CH3OH   1.7435E13   0.0         17.333e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     C_rad/H2/O
      deltaHrxn(T=298K) = -18.596366135272962 kcal/mol

C4H6Oi-13+O=iC4H5OJ(14)+OH    5.0E12      0.0         1.79e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -19.735307371088865 kcal/mol
C4H6Oi-13+O=iC4H5OJ(15)+OH    2850  3.05  3.123e+03   !H_Abstraction
estimate: (Average:)    C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -14.53574171398207 kcal/mol
C4H6Oi-12+O=iC4H5OJ(14)+OH    5700  3.05  3.123e+03   !H_Abstraction
estimate: (Average:)    C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -25.270920553302844 kcal/mol

!C4H6Oi-13+OH=iC4H5OJ(14)+H2O 5.486E12    0.0         5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -35.799294039288895 kcal/mol
C4H6Oi-13+OH=iC4H5OJ(14)+H2O  2.65E12           0.0         -724.19
      !Estimated, based on CH3CHO+OH=H2O+CH3CO
!C4H6Oi-13+OH=iC4H5OJ(15)+H2O 1.991E7           1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
      deltaHrxn(T=298K) = -30.599728382182096 kcal/mol
C4H6Oi-13+OH=iC4H5OJ(15)+H2O  3.12E+06    2.00  -298.757    !Estimate,
based on C3H6+OH=H2O+aC3H5
C4H6Oi-12+OH=iC4H5OJ(14)+H2O  3.982E7           1.75  3.789e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_pri_rad
      deltaHrxn(T=298K) = -41.33490722150286 kcal/mol
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!Following based on Baulch et al.'s CH3CHO+O2=HO2+CH3CO kinetics
C4H6Oi-13+O2=iC4H5OJ(14)+HO2  3.01E13           0.0   39.15e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O2b
      deltaHrxn(T=298K) = 33.89586139116184 kcal/mol
C4H6Oi-13+O2=iC4H5OJ(15)+HO2  1.206E14    0.0   51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 39.09542704826863 kcal/mol
C4H6Oi-12+O2=iC4H5OJ(14)+HO2  2.412E14    0.0   51.87e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O2b
      deltaHrxn(T=298K) = 28.360248208947866 kcal/mol

C4H6Oi-13+HO2=iC4H5OJ(14)+H2O2      5.486E12    0.0         5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_rad/NonDeO
      deltaHrxn(T=298K) = -4.572272470528535 kcal/mol
iC4H5OJ(15)+H2O2=C4H6Oi-13+HO2      2.0305            3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     H2O2
      deltaHrxn(T=298K) = -0.6272931865782638 kcal/mol
C4H6Oi-12+HO2=iC4H5OJ(14)+H2O2      3.9820E7    1.75  3.7894e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_rad/NonDeO
      deltaHrxn(T=298K) = -10.107885652742507 kcal/mol

C3H3OH+H=C3H3OJ(9)+H2   5.06E7      1.98  11.78e+03   !H_Abstraction
exact:      Cd_pri     H_rad        deltaHrxn(T=298K) = -
15.19620816368101 kcal/mol
C3H3OH+H=tSPC(346)+H2   1.3E11      0.82  7.75e+03    !H_Abstraction
exact:      O/H/OneDe     H_rad           deltaHrxn(T=298K) = -
29.304814896103238 kcal/mol

C3H3OH+CH3=C3H3OJ(9)+CH4      6480.0      2.58  14.04e+03
      !H_Abstraction exact:   Cd_pri     C_methyl
      deltaHrxn(T=298K) = -15.987411101740445 kcal/mol
C3H3OH+CH3=tSPC(346)+CH4      90700.0     2.04  10.85e+03
      !H_Abstraction exact:   O/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -30.096017834162673 kcal/mol

C3H3OH+CH2OH=C3H3OJ(9)+CH3OH  4.40555E13  0.0   25.733e+03
      !H_Abstraction estimate: (Average:) Cd_pri     C_rad/H2/O
      deltaHrxn(T=298K) = -7.061295341805263 kcal/mol
C3H3OH+CH2OH=tSPC(346)+CH3OH  136.058           2.7   6.460e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     C_rad/H2/O
      deltaHrxn(T=298K) = -21.169902074227487 kcal/mol

C3H3OH+O=C3H3OJ(9)+OH   7560000.0   1.91  3.74e+03    !H_Abstraction
exact:      Cd_pri     O_atom_triplet           deltaHrxn(T=298K) = -
13.735849759835133 kcal/mol
C3H3OH+O=tSPC(346)+OH   1.00E13           0.0         4.69e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -27.844456492257358 kcal/mol

C3H3OH+OH=C3H3OJ(9)+H2O       1.026E13    0.0   5.94e+03
      !H_Abstraction exact:   Cd_pri     O_pri_rad
      deltaHrxn(T=298K) = -29.79983642803516 kcal/mol
C3H3OH+OH=tSPC(346)+H2O 17.3        3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    O/H/OneDe     O_pri_rad       deltaHrxn(T=298K)
= -43.90844316045739 kcal/mol
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C3H3OH+O2=C3H3OJ(9)+HO2       1.4336E14   0.0         60.01e+03
      !H_Abstraction exact:   Cd_pri     O2b          deltaHrxn(T=298K)
= 39.89531900241557 kcal/mol
!C3H3OH+O2=tSPC(346)+HO2      674422            2.1064      16.1634e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 25.78671226999334 kcal/mol
C3H3OH+O2=tSPC(346)+HO2 1.00E+11    0.0         44.2456e+03
      !H_Abstraction estimate: (Average:) O/H/OneDe     O2b
      deltaHrxn(T=298K) = 44.245582852108726 kcal/mol

C3H3OJ(9)+H2O2=C3H3OH+HO2     28.8  3.1   6.94e+03    !H_Abstraction
estimate: (Average:)    Cd_pri_rad     H2O2           deltaHrxn(T=298K)
= -1.427185140725193 kcal/mol
C3H3OH+HO2=tSPC(346)+H2O2     17.3  3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    O/H/OneDe     O_rad/NonDeO
      deltaHrxn(T=298K) = -12.681421591697031 kcal/mol


!22Jul2010: Butanal chemistry
!C2H5+CH2CO=C4H7OJ(8)   1.926E11    0.041 9.29e+03
      !R_Addition_MultipleBond estimate: (Average:)   C_rad/H2/Cs
Cd/H2_Ck          deltaHrxn(T=298K) = -29.725813212519554 kcal/mol
!CH3CHCHCHO+H=C4H7OJ(13)           2.85E13           0.0
      4.3e+03           !R_Addition_MultipleBond estimate: (Average:)
      Cd/H/De_Cd/H/Nd     H_rad           deltaHrxn(T=298K) = -
26.983283824217736 kcal/mol

!23Jul2010:
!O2+CH2CHO=HO2+CH2CO    1.20E12     0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O2_birad     COpri_Csrad
      deltaHrxn(T=298K) = -14.397364915324221 kcal/mol
O2+C4H7OJ(13)=HO2+CH3CHCHCHO  1.8066E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  O2_birad
C/H2/De_Csrad           deltaHrxn(T=298K) = -22.108287149434442 kcal/mol
O2+C4H7OJ(12)=HO2+CH3CHCHCHO  1.8066E11   0.0   0.0e+03
      !Disproportionation exact:    O2_birad     C/H2/Nd_Csrad
      deltaHrxn(T=298K) = -18.848772296824553 kcal/mol
!CH3CHCHCHO+H=C4H7OJ(12)                   1.000E13    0.0   2.9e+03
      !R_Addition_MultipleBond estimate: (Average:)   Cd/H/Nd_Cd/H/De
H_rad       deltaHrxn(T=298K) = -30.242798676827626 kcal/mol

!26Jul2010: iso-Butanol oxidation chemistry
iBuOH+C4H9Oi2=C4H9Oi3+iBuOH 3.0397882e+06        1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C/H2/CsO     C_rad/Cs3
C4H9Oi2+C4H9Oi3=iBuOH+C4H8O-i3 3.4700000e+14     -0.75000    0.00000
!Disproportionation exact:   C_rad/Cs3     O_Csrad
C4H9Oi3+C4H9Oi3=iBuOH+C4H8O-i3 2.3500000e+12     0.00000     0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     O_Csrad
O2+C4H9Oi2=HO2+C4H8O-i1 2.5399920e+11      0.00000     0.00000
!Disproportionation exact:   O2_birad     Cmethyl_Csrad
C4H9Oi2+C4H9Oi2=iBuOH+C4H8O-i1 1.7160000e+16     -1.10000    0.00000
!Disproportionation exact:   C_rad/Cs3     Cmethyl_Csrad
C4H9Oi3+C4H9Oi2=iBuOH+C4H8O-i1 1.2660000e+15     -0.70000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     Cmethyl_Csrad
O2+C4H9Oi2=HO2+C4H8O-i2 1.8066000e+11      0.00000     0.00000
!Disproportionation exact:   O2_birad     C/H2/Nd_Csrad
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C4H9Oi2+C4H9Oi2=iBuOH+C4H8O-i2 4.3200000e+14     -0.75000    0.00000
!Disproportionation exact:   C_rad/Cs3     C/H2/Nd_Csrad
C4H9Oi3+C4H9Oi2=iBuOH+C4H8O-i2 1.0260000e+14     -0.35000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     C/H2/Nd_Csrad
C4H9Oi3+C4H9Oi3=iBuOH+C4H8O-i2 2.5600000e+13     -0.35000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     C/H/NdNd_Csrad
OH+C4H9Oi2=H2O+C4H8O-i1 1.4460000e+14      0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     O_pri_rad
OH+C4H9Oi2=H2O+C4H8O-i2 4.8200000e+13      0.00000     0.00000
!Disproportionation exact:   O_pri_rad     C/H2/Nd_Csrad
OH+C4H9Oi3=H2O+C4H8O-i2 1.2100000e+13      0.00000     0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     O_pri_rad
OH+C4H9Oi3=H2O+C4H8O-i3 2.4100000e+13      0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
C4H9Oi1+iBuOH=iBuOH+C4H9Oi2 4.2200000e+03        2.51000     8060.00000
       !H_Abstraction exact:   C_rad/H2/Cs     C/H/Cs3
C4H9Oi1+iBuOH=iBuOH+C4H9Oi3 3.0397882e+06        1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cs     C/H2/CsO
C4H9Oi3+C4H9Oi1=C4H8O-i3+iBuOH 2.4100000e+12     0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cs
C4H9Oi2+C4H9Oi1=C4H8O-i1+iBuOH 1.3800000e+14     -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
C4H9Oi1+C4H9Oi1=C4H8O-i1+iBuOH 8.4300000e+11     0.00000     0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cs
C4H9Oi1+C4H9Oi3=C4H8O-i1+iBuOH 2.5600000e+13     -0.35000    0.00000
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad     C_rad/H/CsO
C4H9Oi1+O2=C4H8O-i1+HO2 4.8176000e+10      0.00000     0.00000
!Disproportionation exact:   O2_birad     C/H/NdNd_Csrad
C4H9Oi3+C4H9Oi1=C4H8O-i2+iBuOH 8.4300000e+11     0.00000     0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cs
C4H9Oi2+C4H9Oi1=C4H8O-i2+iBuOH 2.9000000e+12     0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cs
C4H9Oi1+OH=C4H8O-i1+H2O 1.2100000e+13      0.00000     0.00000
!Disproportionation exact:   O_pri_rad     C/H/NdNd_Csrad
C4H9Oi2+CH2OH=iBuOH+CH2O 3.4700000e+14     -0.75000    0.00000
!Disproportionation exact:   C_rad/Cs3     O_Csrad
C4H9Oi3+CH2OH=iBuOH+CH2O 2.3500000e+12     0.00000     0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     O_Csrad
C4H9Oi1+CH2OH=iBuOH+CH2O 2.4100000e+12     0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cs
HO2+C4H9Oi2=H2O2+C4H8O-i1 1.4460000e+14    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Csrad
HO2+C4H9Oi2=H2O2+C4H8O-i2 4.8200000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO     C/H2/Nd_Csrad
HO2+C4H9Oi3=H2O2+C4H8O-i2 1.2100000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
HO2+C4H9Oi3=H2O2+C4H8O-i3 1.2100000e+13    0.00000     0.00000
!Disproportionation exact:   O_rad/NonDeO     O_Csrad
HO2+C4H9Oi1=H2O2+C4H8O-i1 1.2100000e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO
C/H/NdNd_Csrad
C3H6+O2=sC3H5+HO2 3.97E13     0.0   57.29e+03   !H_Abstraction exact:
      No comment  Keq =5.308458700075788E-7     deltaHrxn(T=298K) =
58.103987827981996 kcal/mol
sC3H5+H2O2=C3H6+HO2 2.8800000e+01    3.10000     6940.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     H2O2
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sC3H5+iBuOH=C3H6+C4H9Oi2 1.0200000e+11     0.00000     5300.00000
!H_Abstraction exact:   C/H/Cs3     Cd_rad/NonDeC
!sC3H5+iBuOH=C3H6+C4H9Oi3 1.0200000e+11    0.00000     8820.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     C/H2/CsO
iBuOH+sC3H5=C3H6+C4H9Oi3      2.56e-02    4.09  3.31e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!sC3H5+iBuOH=C3H6+C4H9Oi1 1.0200000e+11    0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     C/H3/Cs
iBuOH+sC3H5=C3H6+C4H9Oi1      1.87e-04    4.87  3.50e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C4H9Oi3+sC3H5=C4H8O-i3+C3H6 3.0100000e+13        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     Cd_rad/NonDeC
C4H9Oi2+sC3H5=C4H8O-i1+C3H6 9.1200000e+14        -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
Cd_rad/NonDeC
C4H9Oi1+sC3H5=C4H8O-i1+C3H6 8.4300000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
Cd_rad/NonDeC
C4H9Oi3+sC3H5=C4H8O-i2+C3H6 8.4300000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
Cd_rad/NonDeC
C4H9Oi2+sC3H5=C4H8O-i2+C3H6 2.4200000e+12        0.00000     0.00000
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
Cd_rad/NonDeC
CH2OH+sC3H5=CH2O+C3H6 3.0100000e+13        0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     Cd_rad/NonDeC
C4H7OJ(79)+iBuOH=C4H8O-i1+C4H9Oi2 2.2900000e+10        0.00000
2880.00000   !H_Abstraction exact:   C/H/Cs3     O_rad/NonDeC
C4H7OJ(79)+iBuOH=C4H8O-i1+C4H9Oi3 2.6681028e+09        0.95000
5644.00000   !H_Abstraction estimate: (Average:)  O_rad/NonDeC
C/H2/CsO
C4H9Oi3+C4H7OJ(79)=C4H8O-i3+C4H8O-i1 2.4100000e+13     0.00000
0.00000      !Disproportionation exact:   O_rad/NonDeC     O_Csrad
C4H9Oi2+C4H7OJ(79)=C4H8O-i1+C4H8O-i1 1.4460000e+14     0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/NonDeC
C4H9Oi1+C4H7OJ(79)=C4H8O-i1+C4H8O-i1 1.2100000e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/NonDeC
C4H9Oi3+C4H7OJ(79)=C4H8O-i2+C4H8O-i1 1.2100000e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/NonDeC
C4H9Oi2+C4H7OJ(79)=C4H8O-i2+C4H8O-i1 4.8200000e+13     0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_rad/NonDeC
C4H7OJ(79)+iBuOH=C4H8O-i1+C4H9Oi1 3.1620000e+11        0.00000
7000.00000   !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
CH2OH+C4H7OJ(79)=CH2O+C4H8O-i1 2.4100000e+13     0.00000     0.00000
!Disproportionation exact:   O_rad/NonDeC     O_Csrad
C4H8O-i1+sC3H5=C4H7OJ(79)+C3H6 1.4400000e+01     3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/NonDeC     Cd_rad/NonDeC
C4H8O-i3+C4H9Oi2=iC4H7OJ(30)+iBuOH 1.6208066e+08       1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C/H/Cs2
C_rad/Cs3
C4H8O-i3+C4H9Oi3=iC4H7OJ(30)+iBuOH 1.6208066e+08       1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C/H/Cs2
C_rad/H/CsO
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C4H9Oi3+iC4H7OJ(30)=C4H8O-i3+C4H8O-i3 3.4700000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/Cs2
C4H9Oi2+iC4H7OJ(30)=C4H8O-i1+C4H8O-i3 1.7160000e+16    -1.10000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/Cs2
C4H9Oi1+iC4H7OJ(30)=C4H8O-i1+C4H8O-i3 1.0800000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/Cs2
C4H8O-i2+C4H9Oi2=iC4H7OJ(30)+iBuOH 1.3605774e+02       2.70083
10460.10417        !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/Cs3
C4H8O-i2+C4H9Oi3=iC4H7OJ(30)+iBuOH 1.3605774e+02       2.70083
10460.10417        !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/CsO
C4H9Oi3+iC4H7OJ(30)=C4H8O-i2+C4H8O-i3 1.0800000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/Cs2
C4H9Oi2+iC4H7OJ(30)=C4H8O-i2+C4H8O-i3 4.3200000e+14    -0.75000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/Cs2
C4H9Oi2+iC4H7OJ(30)=C4H8O-i1+C4H8O-i2 1.4460000e+14    0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C4H9Oi1+iC4H7OJ(30)=C4H8O-i1+C4H8O-i2 1.2100000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/OneDe
C4H9Oi3+iC4H7OJ(30)=C4H8O-i2+C4H8O-i2 1.2100000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/OneDe
C4H9Oi2+iC4H7OJ(30)=C4H8O-i2+C4H8O-i2 4.8200000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_rad/OneDe
C4H8O-i3+C4H9Oi1=iC4H7OJ(30)+iBuOH 1.6208066e+08       1.00444
11128.61111        !H_Abstraction estimate: (Average:)  C/H/Cs2
C_rad/H2/Cs
C4H8O-i2+C4H9Oi1=iC4H7OJ(30)+iBuOH 1.3605774e+02       2.70083
10460.10417        !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
CH2OH+iC4H7OJ(30)=CH2O+C4H8O-i3 3.4700000e+14    -0.75000    0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/Cs2
CH2OH+iC4H7OJ(30)=CH2O+C4H8O-i2 1.7076592e+13    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     O_rad/OneDe
C4H8O-i3+sC3H5=iC4H7OJ(30)+C3H6 7.6354545e+12    0.00000     7725.00000
       !H_Abstraction estimate: (Average:)  C/H/Cs2     Cd_rad/NonDeC
C4H8O-i2+sC3H5=iC4H7OJ(30)+C3H6 1.4400000e+01    3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_rad/NonDeC
C4H8O-i3+C4H7OJ(79)=iC4H7OJ(30)+C4H8O-i1 8.0670536e+08       0.95000
5448.25000   !H_Abstraction estimate: (Average:)  C/H/Cs2
O_rad/NonDeC
C4H8O-i2+C4H7OJ(79)=iC4H7OJ(30)+C4H8O-i1 1.7300000e+01       3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/NonDeC
C4H8O-i2+iC4H7OJ(30)=iC4H7OJ(30)+C4H8O-i3 1.3605774e+02      2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/Cs2
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O2+iC4H7OJ(30)=HO2+C4H6Oi-12 1.2000000e+12       0.00000     0.00000
!Disproportionation estimate: (Average:)  O2_birad     COpri_Csrad
HO2+iC4H7OJ(30)=H2O2+C4H6Oi-12 1.5736900e+12     -0.03782    1039.02297
       !Disproportionation estimate: (Average:)  O_rad/NonDeO
COpri_Csrad
C4H9Oi2+iC4H7OJ(30)=iBuOH+C4H6Oi-12 1.5736900e+12      -0.03782
1039.02297   !Disproportionation estimate: (Average:)  C_rad/Cs3
COpri_Csrad
C4H9Oi3+iC4H7OJ(30)=iBuOH+C4H6Oi-12 1.5736900e+12      -0.03782
1039.02297   !Disproportionation estimate: (Average:)  C_rad/H/CsO
COpri_Csrad
OH+iC4H7OJ(30)=H2O+C4H6Oi-12 1.5736900e+12       -0.03782    1039.02297
       !Disproportionation estimate: (Average:)  O_pri_rad
COpri_Csrad
C4H9Oi1+iC4H7OJ(30)=iBuOH+C4H6Oi-12 1.5736900e+12      -0.03782
1039.02297   !Disproportionation estimate: (Average:)  C_rad/H2/Cs
COpri_Csrad
sC3H5+iC4H7OJ(30)=C3H6+C4H6Oi-12 1.5736900e+12   -0.03782    1039.02297
       !Disproportionation estimate: (Average:)  Cd_rad/NonDeC
COpri_Csrad
C4H7OJ(79)+iC4H7OJ(30)=C4H8O-i1+C4H6Oi-12 1.5736900e+12      -0.03782
1039.02297   !Disproportionation estimate: (Average:)  O_rad/NonDeC
COpri_Csrad
iC4H7OJ(30)+iC4H7OJ(30)=C4H8O-i3+C4H6Oi-12 1.5736900e+12     -0.03782
1039.02297   !Disproportionation estimate: (Average:)  C_rad/Cs2
COpri_Csrad
iC4H7OJ(30)+iC4H7OJ(30)=C4H8O-i2+C4H6Oi-12 1.5736900e+12     -0.03782
1039.02297   !Disproportionation estimate: (Average:)  O_rad/OneDe
COpri_Csrad
O2+C4H7OJ(79)=HO2+C4H6Oi-13 1.8066000e+11        0.00000     0.00000
!Disproportionation estimate: (Average:)  O2_birad     C/H2/De_Orad
HO2+C4H7OJ(79)=H2O2+C4H6Oi-13 1.1401172e+13      -0.07100    -2.16667
!Disproportionation estimate: (Average:)  O_rad/NonDeO     C/H2/De_Orad
C4H9Oi2+C4H7OJ(79)=iBuOH+C4H6Oi-13 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/Cs3
C/H2/De_Orad
C4H9Oi3+C4H7OJ(79)=iBuOH+C4H6Oi-13 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H/CsO
C/H2/De_Orad
OH+C4H7OJ(79)=H2O+C4H6Oi-13 1.1401172e+13        -0.07100    -2.16667
!Disproportionation estimate: (Average:)  O_pri_rad     C/H2/De_Orad
C4H9Oi1+C4H7OJ(79)=iBuOH+C4H6Oi-13 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C_rad/H2/Cs
C/H2/De_Orad
sC3H5+C4H7OJ(79)=C3H6+C4H6Oi-13 1.1401172e+13    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  Cd_rad/NonDeC     C/H2/De_Orad
C4H7OJ(79)+C4H7OJ(79)=C4H8O-i1+C4H6Oi-13 1.1401172e+13       -0.07100
-2.16667     !Disproportionation estimate: (Average:)  O_rad/NonDeC
C/H2/De_Orad
O2+iC4H7OJ(30)=HO2+C4H6Oi-13 2.5399920e+11       0.00000     0.00000
!Disproportionation exact:   O2_birad     Cmethyl_Csrad
HO2+iC4H7OJ(30)=H2O2+C4H6Oi-13 1.4460000e+14     0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/NonDeO     Cmethyl_Csrad
C4H9Oi2+iC4H7OJ(30)=iBuOH+C4H6Oi-13 1.7160000e+16      -1.10000
0.00000      !Disproportionation exact:   C_rad/Cs3     Cmethyl_Csrad
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C4H9Oi3+iC4H7OJ(30)=iBuOH+C4H6Oi-13 1.2660000e+15      -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/CsO
Cmethyl_Csrad
OH+iC4H7OJ(30)=H2O+C4H6Oi-13 1.4460000e+14       0.00000     0.00000
!Disproportionation exact:   O_pri_rad     Cmethyl_Csrad
C4H9Oi1+iC4H7OJ(30)=iBuOH+C4H6Oi-13 1.3800000e+14      -0.35000
0.00000      !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
sC3H5+iC4H7OJ(30)=C3H6+C4H6Oi-13 9.1200000e+14   -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cd_rad/NonDeC
Cmethyl_Csrad
iC4H7OJ(30)+C4H7OJ(79)=C4H8O-i3+C4H6Oi-13 1.1401172e+13      -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C_rad/Cs2
C/H2/De_Orad
C4H7OJ(79)+iC4H7OJ(30)=C4H8O-i1+C4H6Oi-13 1.4460000e+14      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/NonDeC
Cmethyl_Csrad
iC4H7OJ(30)+iC4H7OJ(30)=C4H8O-i3+C4H6Oi-13 1.7160000e+16     -1.10000
0.00000      !Disproportionation estimate: (Average:)  C_rad/Cs2
Cmethyl_Csrad
iC4H7OJ(30)+iC4H7OJ(30)=C4H8O-i2+C4H6Oi-13 1.4460000e+14     0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/OneDe
Cmethyl_Csrad
iC4H7OJ(30)+C4H7OJ(79)=C4H8O-i2+C4H6Oi-13 1.1401172e+13      -0.07100
-2.16667     !Disproportionation estimate: (Average:)  O_rad/OneDe
C/H2/De_Orad
C4H6Oi-12+C4H9Oi2=iC4H5OJ(14)+iBuOH 1.9080000e+13      0.00000
11200.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/Cs3
C4H6Oi-12+C4H9Oi3=iC4H5OJ(14)+iBuOH 3.9629080e+12      0.00000
16850.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H/CsO
C4H6Oi-12+C4H9Oi1=iC4H5OJ(14)+iBuOH 3.3600000e+12      0.00000
12400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
C4H6Oi-12+sC3H5=iC4H5OJ(14)+C3H6 3.3120000e+13   0.00000     7500.00000
       !H_Abstraction exact:   C/H3/Cd     Cd_rad/NonDeC
C4H6Oi-12+C4H7OJ(79)=iC4H5OJ(14)+C4H8O-i1 3.9819553e+07      1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeC
C4H6Oi-12+iC4H7OJ(30)=iC4H5OJ(14)+C4H8O-i3 2.4780000e+12     0.00000
21100.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/Cs2
C4H6Oi-12+iC4H7OJ(30)=iC4H5OJ(14)+C4H8O-i2 3.9819553e+07     1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/OneDe
C4H9Oi3+iC4H5OJ(14)=C4H8O-i3+C4H6Oi-12 1.8100000e+13   0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C4H9Oi2+iC4H5OJ(14)=C4H8O-i1+C4H6Oi-12 1.3740000e+14   -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H9Oi1+iC4H5OJ(14)=C4H8O-i1+C4H6Oi-12 7.8300000e+11   0.00000     -
130.00000    !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
C4H9Oi3+iC4H5OJ(14)=C4H8O-i2+C4H6Oi-12 7.8300000e+11   0.00000     -
130.00000    !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
C4H9Oi2+iC4H5OJ(14)=C4H8O-i2+C4H6Oi-12 2.9000000e+12   0.00000     -
130.00000    !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cd
CH2OH+iC4H5OJ(14)=CH2O+C4H6Oi-12 1.8100000e+13   0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cd
iC4H7OJ(30)+iC4H5OJ(14)=C4H6Oi-12+C4H6Oi-12 1.5736900e+12    -0.03782
1039.02297   !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H2/Cd
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C4H6Oi-13+C4H9Oi2=iC4H5OJ(14)+iBuOH 1.0533755e+08      1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/Cs3
C4H6Oi-13+C4H9Oi3=iC4H5OJ(14)+iBuOH 1.0533755e+08      1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H/CsO
C4H6Oi-13+C4H9Oi1=iC4H5OJ(14)+iBuOH 1.0533755e+08      1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H2/Cs
C4H6Oi-13+sC3H5=iC4H5OJ(14)+C3H6 8.1300000e+10   0.00000     3680.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     Cd_rad/NonDeC
C4H6Oi-13+C4H7OJ(79)=iC4H5OJ(14)+C4H8O-i1 5.4863467e+12      0.00000
5960.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
O_rad/NonDeC
C4H6Oi-13+iC4H7OJ(30)=iC4H5OJ(14)+C4H8O-i3 1.0533755e+08     1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/Cs2
C4H6Oi-13+iC4H7OJ(30)=iC4H5OJ(14)+C4H8O-i2 5.4863467e+12     0.00000
5960.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
O_rad/OneDe
C4H9Oi3+iC4H5OJ(14)=C4H8O-i3+C4H6Oi-13 1.8100000e+14   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
CO_rad/OneDe
C4H9Oi2+iC4H5OJ(14)=C4H8O-i1+C4H6Oi-13 1.4130468e+14   -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
C4H9Oi1+iC4H5OJ(14)=C4H8O-i1+C4H6Oi-13 3.5218932e+12   -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
CO_rad/OneDe
C4H9Oi3+iC4H5OJ(14)=C4H8O-i2+C4H6Oi-13 3.5218932e+12   -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
CO_rad/OneDe
C4H9Oi2+iC4H5OJ(14)=C4H8O-i2+C4H6Oi-13 1.1401172e+13   -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
CO_rad/OneDe
CH2OH+iC4H5OJ(14)=CH2O+C4H6Oi-13 1.8100000e+14   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     CO_rad/OneDe
iC4H7OJ(30)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-12 1.3740000e+14    -0.35000
-130.00000   !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H7OJ(79)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-12 1.1401172e+13     -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C/H2/De_Orad
C_rad/H2/Cd
iC4H7OJ(30)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-13 1.4130468e+14    -0.22972
-1.80556     !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
C4H7OJ(79)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-13 1.1401172e+13     -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C/H2/De_Orad
CO_rad/OneDe
iC4H5OJ(14)+C4H6Oi-12=C4H6Oi-13+iC4H5OJ(14) 2.9158025e+04    2.73500
17885.00000        !H_Abstraction estimate: (Average:)  CO_rad/OneDe
C/H3/Cd
C4H8O-i1+C4H9Oi2=iC4H7OJ(15)+iBuOH 3.0397882e+06       1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/Cs3
C4H8O-i1+C4H9Oi3=iC4H7OJ(15)+iBuOH 3.0397882e+06       1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/H/CsO
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C4H9Oi3+iC4H7OJ(15)=C4H8O-i3+C4H8O-i1 2.3500000e+12    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/OneDeO
C4H9Oi2+iC4H7OJ(15)=C4H8O-i1+C4H8O-i1 1.2660000e+15    -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeO
C4H9Oi1+iC4H7OJ(15)=C4H8O-i1+C4H8O-i1 2.5600000e+13    -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/H/OneDeO
C4H8O-i2+C4H9Oi2=iC4H7OJ(15)+iBuOH 1.9080000e+13       0.00000
11200.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/Cs3
C4H8O-i2+C4H9Oi3=iC4H7OJ(15)+iBuOH 3.9629080e+12       0.00000
16850.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H/CsO
C4H9Oi3+iC4H7OJ(15)=C4H8O-i3+C4H8O-i2 1.8100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C4H9Oi3+iC4H7OJ(15)=C4H8O-i2+C4H8O-i1 2.5600000e+13    -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
C_rad/H/OneDeO
C4H9Oi2+iC4H7OJ(15)=C4H8O-i2+C4H8O-i1 1.0260000e+14    -0.35000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
C_rad/H/OneDeO
C4H9Oi1+iC4H7OJ(15)=C4H8O-i1+C4H8O-i2 7.8300000e+11    0.00000     -
130.00000    !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
C4H9Oi3+iC4H7OJ(15)=C4H8O-i2+C4H8O-i2 7.8300000e+11    0.00000     -
130.00000    !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
C4H9Oi2+iC4H7OJ(15)=C4H8O-i2+C4H8O-i2 2.9000000e+12    0.00000     -
130.00000    !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cd
C4H8O-i1+C4H9Oi1=iC4H7OJ(15)+iBuOH 3.0397882e+06       1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/H2/Cs
C4H8O-i2+C4H9Oi1=iC4H7OJ(15)+iBuOH 3.3600000e+12       0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
CH2OH+iC4H7OJ(15)=CH2O+C4H8O-i1 2.3500000e+12    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/H/OneDeO
CH2OH+iC4H7OJ(15)=CH2O+C4H8O-i2 1.8100000e+13    0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C4H8O-i1+sC3H5=iC4H7OJ(15)+C3H6 1.0200000e+03    3.10000     8820.00000
       !H_Abstraction estimate: (Average:)  C/H2/OneDeO
Cd_rad/NonDeC
C4H8O-i2+sC3H5=iC4H7OJ(15)+C3H6 3.3120000e+13    0.00000     7500.00000
       !H_Abstraction exact:   C/H3/Cd     Cd_rad/NonDeC
C4H8O-i1+C4H7OJ(79)=iC4H7OJ(15)+C4H8O-i1 2.6681028e+09       0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
O_rad/NonDeC
C4H8O-i2+C4H7OJ(79)=iC4H7OJ(15)+C4H8O-i1 3.9819553e+07       1.75000
3789.37500   !H_Abstraction estimate: (Average:)  C/H3/Cd
O_rad/NonDeC
C4H8O-i1+iC4H7OJ(30)=iC4H7OJ(15)+C4H8O-i3 3.0397882e+06      1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/Cs2
C4H8O-i2+iC4H7OJ(30)=iC4H7OJ(15)+C4H8O-i3 2.4780000e+12      0.00000
21100.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/Cs2
C4H8O-i1+iC4H7OJ(30)=iC4H7OJ(15)+C4H8O-i2 2.6681028e+09      0.95000
5644.00000   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
O_rad/OneDe
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iC4H7OJ(15)+C4H8O-i2=C4H8O-i2+iC4H7OJ(30) 1.3605774e+02      2.70083
6460.10417   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/OneDe
iC4H7OJ(30)+iC4H7OJ(15)=C4H6Oi-12+C4H8O-i1 1.5736900e+12     -0.03782
1039.02297   !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H/OneDeO
iC4H7OJ(30)+iC4H7OJ(15)=C4H6Oi-12+C4H8O-i2 1.5736900e+12     -0.03782
1039.02297   !Disproportionation estimate: (Average:)  COpri_Csrad
C_rad/H2/Cd
iC4H7OJ(15)+C4H9Oi1=C4H6Oi-13+iBuOH 2.4100000e+12      0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cs     O_Csrad
iC4H7OJ(15)+C4H9Oi2=C4H6Oi-13+iBuOH 3.4700000e+14      -0.75000
0.00000      !Disproportionation exact:   C_rad/Cs3     O_Csrad
iC4H7OJ(15)+C4H9Oi3=C4H6Oi-13+iBuOH 2.3500000e+12      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/CsO
iC4H7OJ(15)+O2=C4H6Oi-13+HO2 2.2883600e+13       0.00000     0.00000
!Disproportionation exact:   O2_birad     O_Csrad
iC4H7OJ(15)+iC4H7OJ(30)=C4H6Oi-13+C4H8O-i3 3.4700000e+14     -0.75000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/Cs2
iC4H7OJ(30)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i1 1.2660000e+15     -0.70000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeO
C4H7OJ(79)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i1 1.1401172e+13      -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C/H2/De_Orad
C_rad/H/OneDeO
iC4H7OJ(15)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i1 2.3500000e+12     0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/OneDeO
iC4H7OJ(30)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i2 2.2900000e+13     -0.35000
-130.00000   !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H7OJ(79)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i2 1.1401172e+13      -0.07100
-2.16667     !Disproportionation estimate: (Average:)  C/H2/De_Orad
C_rad/H2/Cd
iC4H7OJ(15)+iC4H7OJ(15)=C4H6Oi-13+C4H8O-i2 1.8100000e+13     0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
iC4H7OJ(15)+OH=C4H6Oi-13+H2O 2.4100000e+13       0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
iC4H7OJ(15)+sC3H5=C4H6Oi-13+C3H6 3.0100000e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     Cd_rad/NonDeC
iC4H7OJ(15)+HO2=C4H6Oi-13+H2O2 1.2100000e+13     0.00000     0.00000
!Disproportionation exact:   O_rad/NonDeO     O_Csrad
iC4H7OJ(15)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-12 1.8100000e+13    0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
iC4H7OJ(15)+iC4H5OJ(14)=C4H6Oi-13+C4H6Oi-13 1.8100000e+14    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
CO_rad/OneDe
iC4H7OJ(15)+C4H6Oi-12=C4H8O-i1+iC4H5OJ(14) 9.1200000e+12     0.00000
21400.00000        !H_Abstraction estimate: (Average:)  C_rad/H/OneDeO
C/H3/Cd
iC4H7OJ(15)+C4H6Oi-12=C4H8O-i2+iC4H5OJ(14) 3.4680000e+13     0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C4H8O-i1+iC4H5OJ(14)=iC4H7OJ(15)+C4H6Oi-13 7.5657121e+06     1.95000
16625.00000        !H_Abstraction estimate: (Average:)  C/H2/OneDeO
CO_rad/OneDe
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iC4H7OJ(15)+C4H6Oi-13=C4H8O-i2+iC4H5OJ(14) 1.0533755e+08     1.14500
6325.00000   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
CO/H/OneDe
iC4H7OJ(15)+C4H8O-i1=C4H8O-i2+iC4H7OJ(15) 3.0397882e+06      1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
C/H2/OneDeO

!29JUL2010: Iso-butanol pyrolysis chemistry
!iBuOH+C3H7-2=C4H9Oi3+C3H8 3.0397882e+05   1.88583     12448.33333
!H_Abstraction estimate: (Average:)  C/H2/CsO     C_rad/H/NonDeC
iBuOH+C3H7-2=C3H8+C4H9Oi3     2.12e-06    5.06  4.89e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
CH3OH+C3H7-2=CH2OH+C3H8 9.4074532e+05      1.75273     12532.12121
!H_Abstraction estimate: (Average:)  C/H3/O     C_rad/H/NonDeC
CH2OH+C3H7-2=CH3OH+C3H6 1.7340000e+13      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/O     Cmethyl_Csrad
C3H7-2+C3H7-2=C3H8+C3H6 1.2660000e+15      -0.70000    0.00000
!Disproportionation exact:   C_rad/H/NonDeC     Cmethyl_Csrad
C4H9Oi3+C3H7-2=iBuOH+C3H6 1.2660000e+15    -0.70000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     Cmethyl_Csrad
H+C3H7-2=H2+C3H6 2.1660000e+13       0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
!iBuOH+C3H7-2=C4H9Oi2+C3H8 5.5800000e+01   3.01000     7340.00000
!H_Abstraction exact:   C/H/Cs3     C_rad/H/NonDeC
iBuOH+C3H7-2=C3H8+C4H9Oi2     2.35e-06    4.84  4.27e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C3H7-2+C4H9Oi2=C3H6+iBuOH 1.7160000e+16    -1.10000    0.00000
!Disproportionation exact:   C_rad/Cs3     Cmethyl_Csrad
OH+C3H7-2=H2O+C3H6 1.4460000e+14     0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     O_pri_rad
C4H9Oi1+C3H8=iBuOH+C3H7-2 3.0800000e+03    2.66000     10100.00000
!H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
C3H7-2+C4H9Oi1=C3H6+iBuOH 1.3800000e+14    -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
CH3+C3H7-2=CH4+C3H6 1.3140000e+15    -0.68000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_methyl
CH2OH+C4H9Oi2=CH3OH+C4H8O-i1 1.7340000e+13       0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/O
C3H7-2+C4H9Oi2=C3H8+C4H8O-i1 1.2660000e+15       -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H/NonDeC
H+C4H9Oi2=H2+C4H8O-i1 2.1660000e+13        0.00000     0.00000
!Disproportionation exact:   Cmethyl_Csrad     H_rad
CH3+C4H9Oi2=CH4+C4H8O-i1 1.3140000e+15     -0.68000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_methyl
CH2OH+C4H9Oi1=CH3OH+C4H8O-i1 2.4100000e+11       0.00000     0.00000
!Disproportionation exact:   C_rad/H2/O     C/H/NdNd_Csrad
C3H7-2+C4H9Oi1=C3H8+C4H8O-i1 2.5600000e+13       -0.35000    0.00000
!Disproportionation exact:   C_rad/H/NonDeC     C/H/NdNd_Csrad
H+C4H9Oi1=H2+C4H8O-i1 9.0400000e+11        0.00000     0.00000
!Disproportionation exact:   H_rad     C/H/NdNd_Csrad
CH3+C4H9Oi1=CH4+C4H8O-i1 6.0200000e+12     -0.32000    0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     C_methyl
iC4H8+CH2OH=iC4H7+CH3OH 1.7434638e+13      0.00000     17333.33333
!H_Abstraction estimate: (Average:)  C/H3/Cd     C_rad/H2/O
iC4H8+C3H7-2=iC4H7+C3H8 1.7220000e+12      0.00000     12300.00000
!H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
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!iC4H8+C4H9Oi3=iC4H7+iBuOH 3.9629080e+12   0.00000     16850.00000
!H_Abstraction estimate: (Average:)  C/H3/Cd     C_rad/H/CsO
!iC4H7+iBuOH=iC4H8+C4H9Oi3  .1020E+06 2.0  15253.34   !Ranzi et al.
!iBuOH+iC4H7=iC4H8+C4H9Oi3    1.56e-02    3.71  12.41e+03   !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
iC4H8+C4H9Oi3=iBuOH+iC4H7     2.95e-05    5.07  3.66e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!iC4H8+C4H9Oi2=iC4H7+iBuOH 1.9080000e+13   0.00000     11200.00000
!H_Abstraction exact:   C/H3/Cd     C_rad/Cs3
!iC4H7+iBuOH=iC4H8+C4H9Oi2  .3399E+05 2.0  13592.23   !Ranzi et al.
!iBuOH+iC4H7=iC4H8+C4H9Oi2    1.89e-03    3.55  10.93e+03   !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
iC4H8+C4H9Oi2=iBuOH+iC4H7     8.64e-05    4.52  1.46e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C3H7-2+iC4H7=C3H6+iC4H8 1.3740000e+14      -0.35000    -130.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
!iC4H8+C4H9Oi1=iC4H7+iBuOH 3.3600000e+12   0.00000     12400.00000
!H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
!iC4H7+iBuOH=iC4H8+C4H9Oi1  .2040E+06 2.0  18575.57   !Ranzi et al.
!iBuOH+iC4H7=iC4H8+C4H9Oi1    3.11e-02    3.68  19.13e+03   !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
iC4H8+C4H9Oi1=iBuOH+iC4H7     5.03e-05    4.89  4.32e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
!iC4H7+iBuOH=iC4H8+C4H9Oi4  .3399E+05 2.0  18575.57   !Ranzi et al.
!iC4H8+C4H9Oi4=iBuOH+iC4H7    3.50e+00    3.74  1.45e+03    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
C4H9Oi2+iC4H7=C4H8O-i1+iC4H8 1.3740000e+14       -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H9Oi1+iC4H7=C4H8O-i1+iC4H8 7.8300000e+11       0.00000     -130.00000
       !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
C4H8O-i1+C3H7-2=iC4H7OJ(15)+C3H8 3.0397882e+06   1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/H/NonDeC
C3H7-2+iC4H7OJ(15)=C3H6+C4H8O-i1 1.2660000e+15   -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
C_rad/H/OneDeO
C4H8O-i1+iC4H7=iC4H7OJ(15)+iC4H8 3.0397882e+06   1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C/H2/OneDeO     C_rad/H2/Cd
CH2OH+C4H9Oi3=CH3OH+C4H8O-i2 2.4100000e+11       0.00000     0.00000
!Disproportionation exact:   C_rad/H2/O     C/H/NdNd_Csrad
C3H7-2+C4H9Oi3=C3H8+C4H8O-i2 2.5600000e+13       -0.35000    0.00000
!Disproportionation exact:   C_rad/H/NonDeC     C/H/NdNd_Csrad
H+C4H9Oi3=H2+C4H8O-i2 9.0400000e+11        0.00000     0.00000
!Disproportionation exact:   H_rad     C/H/NdNd_Csrad
CH2OH+C4H9Oi2=CH3OH+C4H8O-i2 9.6400000e+11       0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/O
C3H7-2+C4H9Oi2=C3H8+C4H8O-i2 1.0260000e+14       -0.35000    0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H/NonDeC
H+C4H9Oi2=H2+C4H8O-i2 3.6200000e+12        0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     H_rad
CH3+C4H9Oi3=CH4+C4H8O-i2 6.0200000e+12     -0.32000    0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     C_methyl
CH3+C4H9Oi2=CH4+C4H8O-i2 2.3000000e+13     -0.32000    0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     C_methyl
iC4H7+C4H9Oi3=iC4H8+C4H8O-i2 7.8300000e+11       0.00000     -130.00000
       !Disproportionation exact:   C/H/NdNd_Csrad     C_rad/H2/Cd
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iC4H7+C4H9Oi2=iC4H8+C4H8O-i2 2.9000000e+12       0.00000     -130.00000
       !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cd
C3H7-2+C4H8O-i2=C3H8+iC4H7OJ(15) 1.7220000e+12   0.00000     12300.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
iC4H8+iC4H7OJ(15)=iC4H7+C4H8O-i2 3.4680000e+13   0.00000     21400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
iC4H7OJ(15)+C3H7-2=C4H8O-i2+C3H6 1.3740000e+14   -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C3H6O-enol+CH2OH=C3H5OJ(12)+CH3OH 1.3605774e+02        2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/O
C3H6O-enol+C3H7-2=C3H5OJ(12)+C3H8 1.3605774e+02        2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/NonDeC
C3H6O-enol+C4H9Oi3=C3H5OJ(12)+iBuOH 1.3605774e+02      2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/CsO
C3H6O-enol+C4H9Oi2=C3H5OJ(12)+iBuOH 1.3605774e+02      2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/Cs3
C3H6O-enol+C4H9Oi1=C3H5OJ(12)+iBuOH 1.3605774e+02      2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cs
C3H7-2+C3H5OJ(12)=C3H6+C3H6O-enol 1.4460000e+14        0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C4H9Oi2+C3H5OJ(12)=C4H8O-i1+C3H6O-enol 1.4460000e+14   0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C4H9Oi1+C3H5OJ(12)=C4H8O-i1+C3H6O-enol 1.2100000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/OneDe
!C3H5OJ(12)+iC4H8=C3H6O-enol+iC4H7 3.9819553e+07       1.75000
13789.37500        !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H3/Cd
C3H5OJ(12)+iC4H8=C3H6O-enol+iC4H7   4.51e-07    5.77  12.04e+03   !MRH
CBS-QB3 RRHO calculation w/asymmetric Eckart
C3H5OJ(12)+C4H8O-i1=C3H6O-enol+iC4H7OJ(15) 2.6681028e+09     0.95000
5644.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
C/H2/OneDeO
C3H6O-enol+iC4H7OJ(15)=C3H5OJ(12)+C4H8O-i2 1.3605774e+02     2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cd
C4H9Oi3+C3H5OJ(12)=C4H8O-i2+C3H6O-enol 1.2100000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
O_rad/OneDe
C4H9Oi2+C3H5OJ(12)=C4H8O-i2+C3H6O-enol 4.8200000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
O_rad/OneDe
!C4H9Oi1+C3H6O=iBuOH+C3H5OJ(12) 3.0397882e+06    1.88583     12448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cs     C/H2/OneDeC
C3H6O+C4H9Oi1=iBuOH+C3H5OJ(12)      3.12e-04    4.31  3.39e+03    !MRH
CBS-QB3 RRHO calculation w/asymmetric Eckart
!iBuOH+C3H5OJ(12)=C4H9Oi2+C3H6O 5.4600000e+12    0.00000     21700.00000
       !H_Abstraction exact:   C/H/Cs3     C_rad/H/OneDeC
iBuOH+C3H5OJ(12)=C3H6O+C4H9Oi2      4.85e-04    4.37  9.66e+03    !MRH
CBS-QB3 RRHO calculation w/asymmetric Eckart
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!iBuOH+C3H5OJ(12)=C4H9Oi3+C3H6O 5.4600000e+12    0.00000     20448.33333
       !H_Abstraction estimate: (Average:)  C/H2/CsO     C_rad/H/OneDeC
iBuOH+C3H5OJ(12)=C3H6O+C4H9Oi3      3.68e-03    4.02  7.92e+03    !MRH
CBS-QB3 RRHO calculation w/asymmetric Eckart
CH2OH+C3H6O=CH3OH+C3H5OJ(12) 3.0397882e+06       1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/O     C/H2/OneDeC
C3H7-2+C3H6O=C3H8+C3H5OJ(12) 3.0397882e+06       1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H/NonDeC
C/H2/OneDeC
iC4H8+C3H5OJ(12)=iC4H7+C3H6O 9.1200000e+12       0.00000     21400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H/OneDeC
OH+C3H6O=H2O+C3H5OJ(12) 2.6681028e+09      0.95000     5644.00000
!H_Abstraction estimate: (Average:)  O_pri_rad     C/H2/OneDeC
C3H6O-enol+C3H5OJ(12)=C3H5OJ(12)+C3H6O 1.3605774e+02   2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/OneDeC
CH3+C3H6O=CH4+C3H5OJ(12) 1.4600000e+13     0.00000     14400.00000
!H_Abstraction exact:   C/H2/OneDeC     C_methyl
C4H8O-i1+C3H5OJ(12)=iC4H7OJ(15)+C3H6O 3.0397882e+06    1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C/H2/OneDeO
C_rad/H/OneDeC
!C4H8O-i2+C3H5OJ(12)=iC4H7OJ(15)+C3H6O 9.1200000e+12   0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H/OneDeC
C3H5OJ(12)+C3H7-2=C3H6O+C3H6 1.2660000e+15       -0.70000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
C3H5OJ(12)+C4H9Oi3=C3H6O+C4H8O-i2 2.5600000e+13        -0.35000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H/NdNd_Csrad
C3H5OJ(12)+C4H9Oi2=C3H6O+C4H8O-i1 1.2660000e+15        -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
C3H5OJ(12)+C4H9Oi2=C3H6O+C4H8O-i2 1.0260000e+14        -0.35000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H2/Nd_Csrad
C3H5OJ(12)+C4H9Oi1=C3H6O+C4H8O-i1 2.5600000e+13        -0.35000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
C/H/NdNd_Csrad
C3H7-2+CH2OH=C3H8+CH2O 2.3500000e+12       0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H/NonDeC
iC4H7+CH2OH=iC4H8+CH2O 1.8100000e+13       0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C3H5OJ(12)+CH2OH=C3H6O-enol+CH2O 1.7076592e+13   0.00000     0.00000
!Disproportionation estimate: (Average:)  O_rad/OneDe     O_Csrad
C3H5OJ(12)+CH2OH=C3H6O+CH2O 2.3500000e+12        0.00000     0.00000
!Disproportionation estimate: (Average:)  C_rad/H/OneDeC     O_Csrad
CH2O+C3H7-2=HCO+C3H8 1.0800000e+11   0.00000     6960.00000
!H_Abstraction exact:   CO_pri     C_rad/H/NonDeC
CH2O+C4H9Oi3=HCO+iBuOH 1.0800000e+11       0.00000     6960.00000
!H_Abstraction estimate: (Average:)  CO_pri     C_rad/H/CsO
CH2O+C4H9Oi2=HCO+iBuOH 3.2600000e+09       0.00000     3560.00000
!H_Abstraction exact:   CO_pri     C_rad/Cs3
CH2O+C4H9Oi1=HCO+iBuOH 5.5000000e+03       2.81000     5860.00000
!H_Abstraction exact:   C_rad/H2/Cs     CO_pri
HCO+C4H8O-i1=CH2O+iC4H7OJ(15) 7.5657121e+06      1.95000     16625.00000
       !H_Abstraction estimate: (Average:)  CO_pri_rad     C/H2/OneDeO
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CH2O+iC4H7OJ(15)=HCO+C4H8O-i2 5.5000000e+03      2.81000     5860.00000
       !H_Abstraction estimate: (Average:)  CO_pri     C_rad/H2/Cd
CH2O+C3H5OJ(12)=HCO+C3H6O-enol 6.4825921e+07     1.25000     6595.00000
       !H_Abstraction estimate: (Average:)  CO_pri     O_rad/OneDe
CH2O+C3H5OJ(12)=HCO+C3H6O 1.0800000e+11    0.00000     6960.00000
!H_Abstraction estimate: (Average:)  CO_pri     C_rad/H/OneDeC
C3H7-2+HCO=C3H6+CH2O 1.4130468e+14   -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_pri_rad
C4H9Oi2+HCO=C4H8O-i1+CH2O 1.4130468e+14    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_pri_rad
C4H9Oi1+HCO=C4H8O-i1+CH2O 3.5218932e+12    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad     CO_pri_rad
C4H9Oi3+HCO=C4H8O-i2+CH2O 3.5218932e+12    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H/NdNd_Csrad     CO_pri_rad
C4H9Oi2+HCO=C4H8O-i2+CH2O 1.1401172e+13    -0.07100    -2.16667
!Disproportionation estimate: (Average:)  C/H2/Nd_Csrad     CO_pri_rad
CH2OH+HCO=CH2O+CH2O 1.8100000e+14    0.00000     0.00000
!Disproportionation exact:   CO_pri_rad     O_Csrad
C3H5OJ(12)+C3H5OJ(12)=C3H6O-enol+C3H4O 7.2300000e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/OneDe
Cmethyl_Csrad
CH2OH+C3H5OJ(12)=CH3OH+C3H4O 8.6700000e+12       0.00000     0.00000
!Disproportionation exact:   C_rad/H2/O     Cmethyl_Csrad
C3H7-2+C3H5OJ(12)=C3H8+C3H4O 6.3300000e+14       -0.70000    0.00000
!Disproportionation exact:   C_rad/H/NonDeC     Cmethyl_Csrad
C4H9Oi3+C3H5OJ(12)=iBuOH+C3H4O 6.3300000e+14     -0.70000    0.00000
!Disproportionation estimate: (Average:)  C_rad/H/CsO     Cmethyl_Csrad
H+C3H5OJ(12)=H2+C3H4O 1.0830000e+13        0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
C4H9Oi2+C3H5OJ(12)=iBuOH+C3H4O 8.5800000e+15     -1.10000    0.00000
!Disproportionation exact:   C_rad/Cs3     Cmethyl_Csrad
CH3+C3H5OJ(12)=CH4+C3H4O 6.5700000e+14     -0.68000    0.00000
!Disproportionation exact:   C_methyl     Cmethyl_Csrad
OH+C3H5OJ(12)=H2O+C3H4O 7.2300000e+13      0.00000     0.00000
!Disproportionation exact:   O_pri_rad     Cmethyl_Csrad
C4H9Oi1+C3H5OJ(12)=iBuOH+C3H4O 6.9000000e+13     -0.35000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cs
iC4H7+C3H5OJ(12)=iC4H8+C3H4O 6.8700000e+13       -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
iC4H7OJ(15)+C3H5OJ(12)=C4H8O-i1+C3H4O 6.3300000e+14    -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeO
Cmethyl_Csrad
iC4H7OJ(15)+C3H5OJ(12)=C4H8O-i2+C3H4O 6.8700000e+13    -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C3H5OJ(12)+C3H5OJ(12)=C3H6O+C3H4O 6.3300000e+14        -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
HCO+C3H5OJ(12)=CH2O+C3H4O 7.0652342e+13    -0.22972    -1.80556
!Disproportionation estimate: (Average:)  CO_pri_rad     Cmethyl_Csrad
C3H6+CH2OH=aC3H5+CH3OH 8.7173191e+12       0.00000     17333.33333
!H_Abstraction estimate: (Average:)  C/H3/Cd     C_rad/H2/O
C3H6+C3H7-2=aC3H5+C3H8 8.6100000e+11       0.00000     12300.00000
!H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
C3H7-2+aC3H5=C3H6+C3H6 1.3740000e+14       -0.35000    -130.00000
!Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H9Oi2+aC3H5=C4H8O-i1+C3H6 1.3740000e+14        -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
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C4H9Oi1+aC3H5=C4H8O-i1+C3H6 7.8300000e+11        0.00000     -130.00000
       !Disproportionation exact:   C_rad/H2/Cd     C/H/NdNd_Csrad
aC3H5+iC4H8=C3H6+iC4H7 3.4680000e+13       0.00000     21400.00000
!H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
aC3H5+C4H8O-i1=C3H6+iC4H7OJ(15) 3.0397882e+06    1.88583     9448.33333
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cd     C/H2/OneDeO
C3H6+iC4H7OJ(15)=aC3H5+C4H8O-i2 1.7340000e+13    0.00000     21400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C4H9Oi3+aC3H5=C4H8O-i2+C3H6 7.8300000e+11        0.00000     -130.00000
       !Disproportionation exact:   C_rad/H2/Cd     C/H/NdNd_Csrad
C4H9Oi2+aC3H5=C4H8O-i2+C3H6 2.9000000e+12        0.00000     -130.00000
       !Disproportionation exact:   C_rad/H2/Cd     C/H2/Nd_Csrad
aC3H5+C3H6O-enol=C3H6+C3H5OJ(12) 1.3605774e+02   2.70083     6460.10417
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cd     O/H/OneDe
C3H6+C3H5OJ(12)=aC3H5+C3H6O 4.5600000e+12        0.00000     21400.00000
       !H_Abstraction exact:   C/H3/Cd     C_rad/H/OneDeC
CH2OH+aC3H5=CH2O+C3H6 1.8100000e+13        0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cd     O_Csrad
C3H5OJ(12)+aC3H5=C3H4O+C3H6 6.8700000e+13        -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C3H6O-enol+CH2OH=C3H5O-enol2+CH3OH 8.7173191e+12       0.00000
17333.33333        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H2/O
C3H6O-enol+C3H7-2=C3H5O-enol2+C3H8 8.6100000e+11       0.00000
12300.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
C3H6O-enol+C4H9Oi3=C3H5O-enol2+iBuOH 1.9814540e+12     0.00000
16850.00000        !H_Abstraction estimate: (Average:)  C/H3/Cd
C_rad/H/CsO
C3H6O-enol+C4H9Oi2=C3H5O-enol2+iBuOH 9.5400000e+12     0.00000
11200.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/Cs3
C3H6O-enol+C4H9Oi1=C3H5O-enol2+iBuOH 1.6800000e+12     0.00000
12400.00000        !H_Abstraction exact:   C_rad/H2/Cs     C/H3/Cd
C3H7-2+C3H5O-enol2=C3H6+C3H6O-enol 1.3740000e+14       -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H9Oi2+C3H5O-enol2=C4H8O-i1+C3H6O-enol 1.3740000e+14        -0.35000
-130.00000   !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C4H9Oi1+C3H5O-enol2=C4H8O-i1+C3H6O-enol 7.8300000e+11        0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     C/H/NdNd_Csrad
C3H5O-enol2+iC4H8=C3H6O-enol+iC4H7 3.4680000e+13       0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C3H5O-enol2+C4H8O-i1=C3H6O-enol+iC4H7OJ(15) 3.0397882e+06    1.88583
9448.33333   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
C/H2/OneDeO
C3H6O-enol+iC4H7OJ(15)=C3H5O-enol2+C4H8O-i2 1.7340000e+13    0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C4H9Oi3+C3H5O-enol2=C4H8O-i2+C3H6O-enol 7.8300000e+11        0.00000
-130.00000   !Disproportionation exact:   C_rad/H2/Cd     C/H/NdNd_Csrad
C4H9Oi2+C3H5O-enol2=C4H8O-i2+C3H6O-enol 2.9000000e+12        0.00000
-130.00000   !Disproportionation exact:   C/H2/Nd_Csrad     C_rad/H2/Cd
C3H5O-enol2+C3H6O-enol=C3H6O-enol+C3H5OJ(12) 1.3605774e+02   2.70083
6460.10417   !H_Abstraction estimate: (Average:)  C_rad/H2/Cd
O/H/OneDe
C3H6O-enol+C3H5OJ(12)=C3H5O-enol2+C3H6O 4.5600000e+12        0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H/OneDeC
CH2OH+C3H5O-enol2=CH2O+C3H6O-enol 1.8100000e+13        0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
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C3H5O-enol2+CH2O=C3H6O-enol+HCO 5.5000000e+03    2.81000     5860.00000
       !H_Abstraction estimate: (Average:)  C_rad/H2/Cd     CO_pri
C3H5O-enol2+C4H9Oi1=C3H4O+iBuOH 2.4100000e+12    0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cs     O_Csrad
C3H5O-enol2+C4H9Oi2=C3H4O+iBuOH 3.4700000e+14    -0.75000    0.00000
!Disproportionation exact:   C_rad/Cs3     O_Csrad
C3H5O-enol2+C4H9Oi3=C3H4O+iBuOH 2.3500000e+12    0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     C_rad/H/CsO
C3H5O-enol2+CH2OH=C3H4O+CH3OH 4.8200000e+12      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/O     O_Csrad
C3H5O-enol2+C3H7-2=C3H4O+C3H8 2.3500000e+12      0.00000     0.00000
!Disproportionation exact:   C_rad/H/NonDeC     O_Csrad
C3H5O-enol2+aC3H5=C3H4O+C3H6 1.8100000e+13       0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cd     O_Csrad
C3H5O-enol2+H=C3H4O+H2 6.0300000e+12       0.00000     0.00000
!Disproportionation exact:   H_rad     O_Csrad
C3H5O-enol2+iC4H7=C3H4O+iC4H8 1.8100000e+13      0.00000     0.00000
!Disproportionation exact:   C_rad/H2/Cd     O_Csrad
C3H5O-enol2+OH=C3H4O+H2O 2.4100000e+13     0.00000     0.00000
!Disproportionation exact:   O_pri_rad     O_Csrad
C3H5O-enol2+C3H5OJ(12)=C3H4O+C3H6O-enol 3.4153184e+13        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
O_rad/OneDe
DUP
C3H5O-enol2+C3H5OJ(12)=C3H4O+C3H6O-enol 4.5800000e+13        -0.35000
-130.00000   !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
DUP

C3H5O-enol2+C3H5O-enol2=C3H4O+C3H6O-enol 1.8100000e+13       0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
C3H5O-enol2+CH3=C3H4O+CH4 2.4100000e+12    0.00000     0.00000
!Disproportionation exact:   C_methyl     O_Csrad
C3H5O-enol2+iC4H7OJ(15)=C3H4O+C4H8O-i1 2.3500000e+12   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/OneDeO
C3H5O-enol2+iC4H7OJ(15)=C3H4O+C4H8O-i2 1.8100000e+13   0.00000
0.00000      !Disproportionation exact:   C_rad/H2/Cd     O_Csrad
C3H5O-enol2+C3H5OJ(12)=C3H4O+C3H6O 2.3500000e+12       0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
C_rad/H/OneDeC
C3H5O-enol2+HCO=C3H4O+CH2O 1.8100000e+14   0.00000     0.00000
!Disproportionation exact:   CO_pri_rad     O_Csrad
C3H6O-enol+aC3H5=C3H5O-enol2+C3H6 1.7340000e+13        0.00000
21400.00000        !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cd
C3H4O+CH2OH=C3H3O-enone+CH3OH 1.0533755e+08      1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H2/O
C3H4O+C3H7-2=C3H3O-enone+C3H8 1.0533755e+08      1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H/NonDeC
C3H4O+C4H9Oi3=C3H3O-enone+iBuOH 1.0533755e+08    1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H/CsO
C3H4O+C4H9Oi2=C3H3O-enone+iBuOH 1.0533755e+08    1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/Cs3
C3H4O+CH3=C3H3O-enone+CH4 1.0533755e+08    1.14500     6325.00000
!H_Abstraction estimate: (Average:)  CO/H/OneDe     C_methyl
C3H4O+C4H9Oi1=C3H3O-enone+iBuOH 1.0533755e+08    1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H2/Cs
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C3H4O+iC4H7=C3H3O-enone+iC4H8 1.0533755e+08      1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H2/Cd
C3H3O-enone+C4H8O-i1=C3H4O+iC4H7OJ(15) 7.5657121e+06   1.95000
16625.00000        !H_Abstraction estimate: (Average:)  CO_rad/OneDe
C/H2/OneDeO
C3H4O+iC4H7OJ(15)=C3H3O-enone+C4H8O-i2 1.0533755e+08   1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H2/Cd
!C3H4O+C3H5OJ(12)=C3H3O-enone+C3H6O-enol 5.4863467e+12       0.00000
5960.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
O_rad/OneDe
C3H4O+C3H5OJ(12)=C3H3O-enone+C3H6O 1.0533755e+08       1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H/OneDeC
C3H4O+HCO=C3H3O-enone+CH2O 4.2583018e+08   1.18432     11145.00000
!H_Abstraction estimate: (Average:)  CO/H/OneDe     CO_pri_rad
C3H7-2+C3H3O-enone=C3H6+C3H4O 1.4130468e+14      -0.22972    -1.80556
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     CO_rad/OneDe
C4H9Oi2+C3H3O-enone=C4H8O-i1+C3H4O 1.4130468e+14       -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
C4H9Oi1+C3H3O-enone=C4H8O-i1+C3H4O 3.5218932e+12       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
CO_rad/OneDe
C4H9Oi3+C3H3O-enone=C4H8O-i2+C3H4O 3.5218932e+12       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H/NdNd_Csrad
CO_rad/OneDe
C4H9Oi2+C3H3O-enone=C4H8O-i2+C3H4O 1.1401172e+13       -0.07100    -
2.16667      !Disproportionation estimate: (Average:)  C/H2/Nd_Csrad
CO_rad/OneDe
CH2OH+C3H3O-enone=CH2O+C3H4O 1.8100000e+14       0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     CO_rad/OneDe
C3H5O-enol2+C3H3O-enone=C3H4O+C3H4O 1.8100000e+14      0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
CO_rad/OneDe
C3H5OJ(12)+C3H3O-enone=C3H4O+C3H4O 7.0652342e+13       -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
C3H4O+aC3H5=C3H3O-enone+C3H6 1.0533755e+08       1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H2/Cd
C3H4O+C3H5O-enol2=C3H3O-enone+C3H6O-enol 1.0533755e+08       1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H2/Cd
iBuOH+C2H3=C4H9Oi1+C2H4 3.0215822e+13      0.00000     9175.00000
!H_Abstraction estimate: (Average:)  C/H3/Cs     Cd_pri_rad
!iBuOH+C2H3=C4H9Oi2+C2H4 8.9500000e+13     0.00000     6200.00000
!H_Abstraction exact:   C/H/Cs3     Cd_pri_rad
iBuOH+C2H3=C2H4+C4H9Oi2       5.49e+00    3.33  6.30e+02    !MRH CBS-QB3
RRHO calculation w/asymmetric Eckart
iBuOH+C2H3=C4H9Oi3+C2H4 1.0200000e+03      3.10000     8820.00000
!H_Abstraction estimate: (Average:)  C/H2/CsO     Cd_pri_rad
CH3OH+C2H3=CH2OH+C2H4 1.5107911e+13        0.00000     9175.00000
!H_Abstraction estimate: (Average:)  C/H3/O     Cd_pri_rad
C3H8+C2H3=C3H7-2+C2H4 1.0200000e+03        3.10000     8820.00000
!H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
C3H6+C2H3=aC3H5+C2H4 2.3190000e+13   0.00000     7500.00000
!H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
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iC4H8+C2H3=iC4H7+C2H4 4.6380000e+13        0.00000     7500.00000
!H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
C3H6O-enol+C2H3=C3H5OJ(12)+C2H4 1.4400000e+01    3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_pri_rad
C3H6O-enol+C2H3=C3H5O-enol2+C2H4 2.3190000e+13   0.00000     7500.00000
       !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
C4H8O-i1+C2H3=iC4H7OJ(15)+C2H4 1.0200000e+03     3.10000     8820.00000
       !H_Abstraction estimate: (Average:)  C/H2/OneDeO     Cd_pri_rad
C4H8O-i2+C2H3=iC4H7OJ(15)+C2H4 4.6380000e+13     0.00000     7500.00000
       !H_Abstraction exact:   Cd_pri_rad     C/H3/Cd
C3H6O+C2H3=C3H5OJ(12)+C2H4 1.0200000e+03   3.10000     8820.00000
!H_Abstraction estimate: (Average:)  C/H2/OneDeC     Cd_pri_rad
CH2O+C2H3=HCO+C2H4 5.4200000e+03     2.81000     5860.00000
!H_Abstraction exact:   CO_pri     Cd_pri_rad
C3H4O+C2H3=C3H3O-enone+C2H4 8.1300000e+10        0.00000     3680.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     Cd_pri_rad
C2H3+CH2OH=C2H4+CH2O 3.0100000e+13   0.00000     0.00000
!Disproportionation exact:   O_Csrad     Cd_pri_rad
C2H3+C3H7-2=C2H4+C3H6 9.1200000e+14        -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C2H3+C4H9Oi3=C2H4+C4H8O-i2 8.4300000e+11   0.00000     0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     Cd_pri_rad
C2H3+C4H9Oi2=C2H4+C4H8O-i1 9.1200000e+14   -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C2H3+C4H9Oi2=C2H4+C4H8O-i2 2.4200000e+12   0.00000     0.00000
!Disproportionation exact:   C/H2/Nd_Csrad     Cd_pri_rad
C2H3+C4H9Oi1=C2H4+C4H8O-i1 8.4300000e+11   0.00000     0.00000
!Disproportionation exact:   C/H/NdNd_Csrad     Cd_pri_rad
C2H3+C3H5OJ(12)=C2H4+C3H4O 4.5600000e+14   -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C2H3+C3H5O-enol2=C2H4+C3H4O 3.0100000e+13        0.00000     0.00000
!Disproportionation exact:   O_Csrad     Cd_pri_rad
C4H8O-i2+C3H7-2=iC4H7OJ(30)+C3H8 1.3605774e+02   2.70083     6460.10417
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H/NonDeC
iC4H7OJ(30)+iC4H8=C4H8O-i2+iC4H7 3.9819553e+07   1.75000     3789.37500
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     C/H3/Cd
C3H7-2+iC4H7OJ(30)=C3H6+C4H8O-i2 1.4460000e+14   0.00000     0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad     O_rad/OneDe
!C4H8O-i2+C3H5OJ(12)=iC4H7OJ(30)+C3H6O-enol 1.7300000e+01    3.40000
-1140.00000        !H_Abstraction estimate: (Average:)  O/H/OneDe
O_rad/OneDe
C4H8O-i2+C3H5OJ(12)=iC4H7OJ(30)+C3H6O 1.3605774e+02    2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H/OneDeC
iC4H7OJ(30)+CH2O=C4H8O-i2+HCO 6.4825921e+07      1.25000     6595.00000
       !H_Abstraction estimate: (Average:)  O_rad/OneDe     CO_pri
C3H5O-enol2+iC4H7OJ(30)=C3H4O+C4H8O-i2 1.7076592e+13   0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
O_rad/OneDe
C3H5OJ(12)+iC4H7OJ(30)=C3H4O+C4H8O-i2 7.2300000e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
O_rad/OneDe
C4H8O-i2+aC3H5=iC4H7OJ(30)+C3H6 1.3605774e+02    2.70083     6460.10417
       !H_Abstraction estimate: (Average:)  O/H/OneDe     C_rad/H2/Cd
C4H8O-i2+C3H5O-enol2=iC4H7OJ(30)+C3H6O-enol 1.3605774e+02    2.70083
6460.10417   !H_Abstraction estimate: (Average:)  O/H/OneDe
C_rad/H2/Cd
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iC4H7OJ(30)+C3H4O=C4H8O-i2+C3H3O-enone 5.4863467e+12   0.00000
5960.00000   !H_Abstraction estimate: (Average:)  O_rad/OneDe
CO/H/OneDe
C4H8O-i2+C2H3=iC4H7OJ(30)+C2H4 1.4400000e+01     3.10000     6940.00000
       !H_Abstraction estimate: (Average:)  O/H/OneDe     Cd_pri_rad
CH2OH+iC4H7OJ(15)=CH3OH+C4H6Oi-13 4.8200000e+12        0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/O
C3H7-2+iC4H7OJ(15)=C3H8+C4H6Oi-13 2.3500000e+12        0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H/NonDeC
H+iC4H7OJ(15)=H2+C4H6Oi-13 6.0300000e+12   0.00000     0.00000
!Disproportionation exact:   O_Csrad     H_rad
CH3+iC4H7OJ(15)=CH4+C4H6Oi-13 2.4100000e+12      0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_methyl
iC4H7+iC4H7OJ(15)=iC4H8+C4H6Oi-13 1.8100000e+13        0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C3H5OJ(12)+iC4H7OJ(15)=C3H6O-enol+C4H6Oi-13 1.7076592e+13    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/OneDe
O_Csrad
C3H5OJ(12)+iC4H7OJ(15)=C3H6O+C4H6Oi-13 2.3500000e+12   0.00000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
O_Csrad
HCO+iC4H7OJ(15)=CH2O+C4H6Oi-13 1.8100000e+14     0.00000     0.00000
!Disproportionation exact:   O_Csrad     CO_pri_rad
aC3H5+iC4H7OJ(15)=C3H6+C4H6Oi-13 1.8100000e+13   0.00000     0.00000
!Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C3H5O-enol2+iC4H7OJ(15)=C3H6O-enol+C4H6Oi-13 1.8100000e+13   0.00000
0.00000      !Disproportionation exact:   O_Csrad     C_rad/H2/Cd
C3H3O-enone+iC4H7OJ(15)=C3H4O+C4H6Oi-13 1.8100000e+14        0.00000
0.00000      !Disproportionation estimate: (Average:)  CO_rad/OneDe
O_Csrad
C2H3+iC4H7OJ(15)=C2H4+C4H6Oi-13 3.0100000e+13    0.00000     0.00000
!Disproportionation exact:   O_Csrad     Cd_pri_rad
CH2OH+iC4H7OJ(30)=CH3OH+C4H6Oi-13 1.7340000e+13        0.00000
0.00000      !Disproportionation exact:   C_rad/H2/O     Cmethyl_Csrad
C3H7-2+iC4H7OJ(30)=C3H8+C4H6Oi-13 1.2660000e+15        -0.70000
0.00000      !Disproportionation exact:   C_rad/H/NonDeC
Cmethyl_Csrad
H+iC4H7OJ(30)=H2+C4H6Oi-13 2.1660000e+13   0.00000     0.00000
!Disproportionation exact:   H_rad     Cmethyl_Csrad
CH3+iC4H7OJ(30)=CH4+C4H6Oi-13 1.3140000e+15      -0.68000    0.00000
!Disproportionation exact:   C_methyl     Cmethyl_Csrad
iC4H7+iC4H7OJ(30)=iC4H8+C4H6Oi-13 1.3740000e+14        -0.35000    -
130.00000    !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C3H5OJ(12)+iC4H7OJ(30)=C3H6O-enol+C4H6Oi-13 1.4460000e+14    0.00000
0.00000      !Disproportionation estimate: (Average:)  O_rad/OneDe
Cmethyl_Csrad
C3H5OJ(12)+iC4H7OJ(30)=C3H6O+C4H6Oi-13 1.2660000e+15   -0.70000
0.00000      !Disproportionation estimate: (Average:)  C_rad/H/OneDeC
Cmethyl_Csrad
HCO+iC4H7OJ(30)=CH2O+C4H6Oi-13 1.4130468e+14     -0.22972    -1.80556
!Disproportionation estimate: (Average:)  CO_pri_rad     Cmethyl_Csrad
aC3H5+iC4H7OJ(30)=C3H6+C4H6Oi-13 1.3740000e+14   -0.35000    -130.00000
       !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
C3H5O-enol2+iC4H7OJ(30)=C3H6O-enol+C4H6Oi-13 1.3740000e+14   -0.35000
-130.00000   !Disproportionation exact:   Cmethyl_Csrad     C_rad/H2/Cd
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C3H3O-enone+iC4H7OJ(30)=C3H4O+C4H6Oi-13 1.4130468e+14        -0.22972
-1.80556     !Disproportionation estimate: (Average:)  CO_rad/OneDe
Cmethyl_Csrad
C2H3+iC4H7OJ(30)=C2H4+C4H6Oi-13 9.1200000e+14    -0.70000    0.00000
!Disproportionation exact:   Cmethyl_Csrad     Cd_pri_rad
C4H6Oi-13+C3H7-2=iC4H5OJ(14)+C3H8 1.0533755e+08        1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H/NonDeC
C4H6Oi-13+iC4H7=iC4H5OJ(14)+iC4H8 1.0533755e+08        1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H2/Cd
C4H6Oi-13+C3H5OJ(12)=iC4H5OJ(14)+C3H6O-enol 5.4863467e+12    0.00000
5960.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
O_rad/OneDe
C4H6Oi-13+C3H5OJ(12)=iC4H5OJ(14)+C3H6O 1.0533755e+08   1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H/OneDeC
C4H6Oi-13+HCO=iC4H5OJ(14)+CH2O 4.2583018e+08     1.18432     11145.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     CO_pri_rad
C4H6Oi-13+aC3H5=iC4H5OJ(14)+C3H6 1.0533755e+08   1.14500     6325.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     C_rad/H2/Cd
C4H6Oi-13+C3H5O-enol2=iC4H5OJ(14)+C3H6O-enol 1.0533755e+08   1.14500
6325.00000   !H_Abstraction estimate: (Average:)  CO/H/OneDe
C_rad/H2/Cd
C4H6Oi-13+C3H3O-enone=iC4H5OJ(14)+C3H4O 4.2583018e+08        1.18432
11145.00000        !H_Abstraction estimate: (Average:)  CO/H/OneDe
CO_rad/OneDe
C4H6Oi-13+C2H3=iC4H5OJ(14)+C2H4 8.1300000e+10    0.00000     3680.00000
       !H_Abstraction estimate: (Average:)  CO/H/OneDe     Cd_pri_rad
C3H7-2+iC4H5OJ(14)=C3H6+C4H6Oi-13 1.4130468e+14        -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
C3H5O-enol2+iC4H5OJ(14)=C3H4O+C4H6Oi-13 1.8100000e+14        0.00000
0.00000      !Disproportionation estimate: (Average:)  O_Csrad
CO_rad/OneDe
C3H5OJ(12)+iC4H5OJ(14)=C3H4O+C4H6Oi-13 7.0652342e+13   -0.22972    -
1.80556      !Disproportionation estimate: (Average:)  Cmethyl_Csrad
CO_rad/OneDe
sC3H5+CH3OH=C3H6+CH2OH 1.5107911e+13       0.00000     9175.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     C/H3/O
sC3H5+C3H8=C3H6+C3H7-2 1.0200000e+03       3.10000     8820.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     C/H2/NonDeC
C3H7-2+sC3H5=C3H6+C3H6 9.1200000e+14       -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
Cd_rad/NonDeC
sC3H5+C3H6O=C3H6+C3H5OJ(12) 1.0200000e+03        3.10000     8820.00000
       !H_Abstraction estimate: (Average:)  Cd_rad/NonDeC
C/H2/OneDeC
sC3H5+CH2O=C3H6+HCO 5.4200000e+03    2.81000     5860.00000
!H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     CO_pri
C3H5O-enol2+sC3H5=C3H4O+C3H6 3.0100000e+13       0.00000     0.00000
!Disproportionation estimate: (Average:)  O_Csrad     Cd_rad/NonDeC
C3H5OJ(12)+sC3H5=C3H4O+C3H6 4.5600000e+14        -0.70000    0.00000
!Disproportionation estimate: (Average:)  Cmethyl_Csrad
Cd_rad/NonDeC
sC3H5+C3H6=C3H6+aC3H5 1.6560000e+13        0.00000     7500.00000
!H_Abstraction exact:   C/H3/Cd     Cd_rad/NonDeC
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sC3H5+C3H6O-enol=C3H6+C3H5O-enol2 1.6560000e+13        0.00000
7500.00000   !H_Abstraction exact:   C/H3/Cd     Cd_rad/NonDeC
sC3H5+C3H4O=C3H6+C3H3O-enone 8.1300000e+10       0.00000     3680.00000
       !H_Abstraction estimate: (Average:)  Cd_rad/NonDeC     CO/H/OneDe
C3H6+C2H3=sC3H5+C2H4 8.4200000e-01   3.50000     9670.00000
!H_Abstraction exact:   Cd_pri_rad     Cd/H/NonDeC

!12/Aug/2010
H+nC3H7OH=H2+C3H7O-N2   2.6E8 1.69  4.78e+03    !H_Abstraction exact:
      C/H2/NonDeC     H_rad         deltaHrxn(T=298K) = -
5.747070626195374 kcal/mol
CH3+nC3H7OH=CH4+C3H7O-N2      2900000.0   1.77  8.53e+03
      !H_Abstraction exact:   C/H2/NonDeC     C_methyl
      deltaHrxn(T=298K) = -6.5382735642548155 kcal/mol
CH3+C3H6O=CH4+C3H5OJ(13)      834000.0    1.9   11.05e+03
      !H_Abstraction exact:   C/H3/Cs     C_methyl
      deltaHrxn(T=298K) = -3.8886153075801744 kcal/mol
C4H9Oi1+nC3H7OH=iBuOH+C3H7O-N2      3079.999999999999 2.66  10.1e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-4(2)3-5/h4-
5H,1,3H2,2H3     C/H2/NonDeC        deltaHrxn(T=298K) = -
3.7093053116249948 kcal/mol
iBuOH+C3H7O-N2=C4H9Oi2+nC3H7OH      55.79999999999998 3.01  7.34e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H10O/c1-4(2)3-5/h4-
5H,3H2,1-2H3/beta     C_rad/H/NonDeC      deltaHrxn(T=298K) = -
0.9501289924835632 kcal/mol
iBuOH+C3H7O-N2=C4H9Oi3+nC3H7OH      2.12E-6     5.06  4.89e+03
      !H_Abstraction exact:   InChI=1/C4H10O/c1-4(2)3-5/h4-5H,3H2,1-
2H3/alpha     C_rad/H/NonDeC        deltaHrxn(T=298K) = -
2.2499438476809317 kcal/mol
C4H9Oi4+nC3H7OH=iBuOH+C3H7O-N2      1.4500000000000012E11   0.0
      4.57e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
4(2)3-5/h4H,3H2,1-2H3     C/H2/NonDeC           deltaHrxn(T=298K) = -
6.209339826670778 kcal/mol
C4H9Oi1+C3H6O=iBuOH+C3H5OJ(13)      1977.0      2.71  12.92e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-4(2)3-5/h4-
5H,1,3H2,2H3     C/H3/Cs      deltaHrxn(T=298K) = -1.0596470549503607
kcal/mol
iBuOH+C3H5OJ(13)=C4H9Oi2+C3H6O      4220.000000000002 2.51  8.06e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H10O/c1-4(2)3-5/h4-
5H,3H2,1-2H3/beta     C_rad/H2/Cs         deltaHrxn(T=298K) = -
3.5997872491581973 kcal/mol
iBuOH+C3H5OJ(13)=C4H9Oi3+C3H6O      3039788.1828314937
      1.8858333333333335      9.448333333333334e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H10O/c1-4(2)3-5/h4-5H,3H2,1-2H3/alpha
C_rad/H2/Cs       deltaHrxn(T=298K) = -4.899602104355566 kcal/mol
C4H9Oi4+C3H6O=iBuOH+C3H5OJ(13)      1.581E11    0.0   7.0e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-4(2)3-
5/h4H,3H2,1-2H3     C/H3/Cs         deltaHrxn(T=298K) = -
3.559681569996144 kcal/mol
iC4H8+C3H7O-N2=iC4H7+nC3H7OH  1.7219999999999978E12   0.0   12.3e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H8/c1-4(2)3/h1H2,2-
3H3     C_rad/H/NonDeC        deltaHrxn(T=298K) = -10.249029426399652
kcal/mol
iC4H8+C3H5OJ(13)=iC4H7+C3H6O  5.0340000000000036E-5   4.89  4.32e+03
      !H_Abstraction exact:   InChI=1/C4H8/c1-4(2)3/h1H2,2-3H3
C_rad/H2/Cs       deltaHrxn(T=298K) = -12.89868768307429 kcal/mol
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OH+nC3H7OH=H2O+C3H7O-N2 7900000.0   1.9   0.16e+03    !H_Abstraction
exact:      C/H2/NonDeC     O_pri_rad           deltaHrxn(T=298K) = -
20.350698890549545 kcal/mol
OH+C3H6O=H2O+C3H5OJ(13) 3600000.0   2.0   0.86e+03    !H_Abstraction
exact:      C/H3/Cs     O_pri_rad         deltaHrxn(T=298K) = -
17.701040633874896 kcal/mol
pC3H5+nC3H7OH=C3H6+C3H7O-N2   1020.0      3.1   8.82e+03
      !H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
      deltaHrxn(T=298K) = -12.74855942513603 kcal/mol
sC3H5+nC3H7OH=C3H6+C3H7O-N2   1019.9999999999998      3.1   8.82e+03
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C/H2/NonDeC
      deltaHrxn(T=298K) = -10.548784046029759 kcal/mol
C3H6+C3H7O-N2=aC3H5+nC3H7OH   8.61E11     0.0   12.3e+03
      !H_Abstraction exact:   C/H3/Cd     C_rad/H/NonDeC
      deltaHrxn(T=298K) = -10.24902937744941 kcal/mol
pC3H5+C3H6O=C3H6+C3H5OJ(13)   2.3189999999999996E13   0.0   7.5e+03
      !H_Abstraction estimate: (Average:) Cd_pri_rad     C/H3/Cs
      deltaHrxn(T=298K) = -10.098901168461396 kcal/mol
sC3H5+C3H6O=C3H6+C3H5OJ(13)   2.3189999999999996E13   0.0   7.5e+03
      !H_Abstraction estimate: (Average:) Cd_rad/NonDeC     C/H3/Cs
      deltaHrxn(T=298K) = -7.899125789355118 kcal/mol
C3H6+C3H5OJ(13)=aC3H5+C3H6O   1.68E12     0.0   12.4e+03
      !H_Abstraction exact:   C/H3/Cd     C_rad/H2/Cs
      deltaHrxn(T=298K) = -12.898687634124045 kcal/mol
C2H3+nC3H7OH=C2H4+C3H7O-N2    1020.0      3.1   8.82e+03
      !H_Abstraction exact:   C/H2/NonDeC     Cd_pri_rad
      deltaHrxn(T=298K) = -12.73394351199385 kcal/mol
C2H3+C3H6O=C2H4+C3H5OJ(13)    2.3189999999999996E13   0.0   7.5e+03
      !H_Abstraction estimate: (Average:) Cd_pri_rad     C/H3/Cs
      deltaHrxn(T=298K) = -10.084285255319216 kcal/mol
C2H5+nC3H7OH=C2H6+C3H7O-N2    3080.0      2.66  10.1e+03
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
      deltaHrxn(T=298K) = -2.2903503366677427 kcal/mol

nC3H7OH+OH=C3H7O-N1+H2O 3600000.0   2.0   0.86e+03    !H_Abstraction
exact:      C/H3/Cs     O_pri_rad         deltaHrxn(T=298K) = -
17.221334319105253 kcal/mol
nC3H7OH+OH=HOCHC2H5+H2O 2.6681027652763863E9    0.95  5.644e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_pri_rad
      deltaHrxn(T=298K) = -23.600416519246814 kcal/mol
nC3H7OH+O=C3H7O-N1+OH   2850.0      3.05  3.123e+03   !H_Abstraction
exact:      C/H3/Cs     O_atom_triplet          deltaHrxn(T=298K) = -
1.157347650905228 kcal/mol
nC3H7OH+O=C3H7O-N2+OH   47800.0     2.71  2.11e+03    !H_Abstraction
exact:      C/H2/NonDeC     O_atom_triplet      deltaHrxn(T=298K) = -
4.286712222349509 kcal/mol
nC3H7OH+O=HOCHC2H5+OH   47800.00000000004 2.71  2.11e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_atom_triplet
      deltaHrxn(T=298K) = -7.536429851046794 kcal/mol
nC3H7OH+O2=C3H7O-N1+HO2 1.206E14    0.0   51.87e+03   !H_Abstraction
exact:      C/H3/Cs     O2b         deltaHrxn(T=298K) =
52.47382111134548 kcal/mol
nC3H7OH+O2=C3H7O-N2+HO2 1.588E14    0.0   47.69e+03   !H_Abstraction
exact:      C/H2/NonDeC     O2b           deltaHrxn(T=298K) =
49.3444565399012 kcal/mol
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nC3H7OH+O2=HOCHC2H5+HO2 1.5880000000000028E14   0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O2b
      deltaHrxn(T=298K) = 46.09473891120392 kcal/mol
C3H7O-N1+H2O2=nC3H7OH+HO2     2.0304986547865194      3.2899999999999996
      1.0725e+03  !H_Abstraction exact:   H2O2     C_rad/H2/Cs
      deltaHrxn(T=298K) = -14.005687249655104 kcal/mol
C3H7O-N2+H2O2=nC3H7OH+HO2     1.1411449715339146      3.283333333333333
      0.8766666666666666e+03  !H_Abstraction exact:   H2O2
C_rad/H/NonDeC          deltaHrxn(T=298K) = -10.876322678210826 kcal/mol
HOCHC2H5+H2O2=nC3H7OH+HO2     2.97  3.39  1.4e+03     !H_Abstraction
exact:      H2O2     C_rad/H/CsO          deltaHrxn(T=298K) = -
7.626605049513536 kcal/mol

!August 26, 2010
aC3H5+H=H2+aC3H4  1.81e+13    0.0   0.0   ! W.Tsang,
J.Phys.Chem.Ref.Data 20 221-273 (1991)

C4H8O-enol+CH3=C4H7OJ(9)+CH4  834000.0    1.9   11.05e+03
      !H_Abstraction exact:   C/H3/Cs     C_methyl
      deltaHrxn(T=298K) = -3.7094251478804896 kcal/mol
C4H8O-enol+OH=C4H7OJ(9)+H2O   3600000.0   2.0   0.86e+03
      !H_Abstraction exact:   C/H3/Cs     O_pri_rad
      deltaHrxn(T=298K) = -18.118196845433665 kcal/mol
C4H8O-enol+O=C4H7OJ(9)+OH     2850.0      3.05  3.123e+03
      !H_Abstraction exact:   C/H3/Cs     O_atom_triplet
      deltaHrxn(T=298K) = -1.2300975028686914 kcal/mol
C4H8O-enol+O2=C4H7OJ(9)+HO2   1.206E14    0.0   51.87e+03
      !H_Abstraction exact:   C/H3/Cs     O2b         deltaHrxn(T=298K)
= 15.968230480871664 kcal/mol
C4H7OJ(9)+H2O2=C4H8O-enol+HO2 2.0305      3.29  1.0725e+03
      !H_Abstraction exact:   H2O2     C_rad/H2/Cs
      deltaHrxn(T=298K) = -15.968227972968343 kcal/mol

OH+C4H9O-1=C4H8O-enol3+H2O    2.41e+13    0.0   0.0
OH+C4H9O-2=C4H8O-enol3+H2O    2.41e+13    0.0   0.0
OH+C4H9O-2=C4H8O-enol2+H2O    2.41e+13    0.0   0.0
OH+C4H9O-3=C4H8O-enol2+H2O    2.41e+13    0.0   0.0
OH+C4H9O-3=C4H8O-enol+H2O     2.41e+13    0.0   0.0
OH+C4H9O-4=C4H8O-enol+H2O     2.41e+13    0.0   0.0

H+C4H7O_1_2=H2+CH3CHCHCHO     6.03E12     0.0   0.0e+03
      !Disproportionation exact:    H_rad     O_Csrad
      deltaHrxn(T=298K) = -68.44232897716294 kcal/mol
OH+C4H7O_1_2=H2O+CH3CHCHCHO   2.41E13     0.0   0.0e+03
      !Disproportionation exact:    O_pri_rad     O_Csrad
      deltaHrxn(T=298K) = -86.56138495985259 kcal/mol

C4H6-13+OH=iC4H5+H2O    2.22e+06    2.0   1.45e+03    !H_Abstraction
estimate: (Average:)    Cd/H/OneDe     O_pri_rad      deltaHrxn(T=298K)
= -19.418211562905718 kcal/mol
HO2+C4H7O_1_2=H2O2+CH3CHCHCHO 1.21E13     0.0   0.0e+03
      !Disproportionation exact:    O_rad/NonDeO     O_Csrad
      deltaHrxn(T=298K) = -52.47496014145057 kcal/mol

C4H4-123+H=iC4H3+H2           1.012E8           1.98  11.78e+03
      !H_Abstraction exact:   Cd_pri     H_rad        deltaHrxn(T=298K)
= -12.097936614005523 kcal/mol
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C4H4-123+OH=iC4H3+H2O   2.052E13    0.0         5.94e+03
      !H_Abstraction exact:   Cd_pri     O_pri_rad
      deltaHrxn(T=298K) = -30.216992596695157 kcal/mol
C4H4-123+CH3=iC4H3+CH4  12960.0           2.58  14.04e+03
      !H_Abstraction exact:   Cd_pri     C_methyl
      deltaHrxn(T=298K) = -15.808220899141968 kcal/mol
C4H4-123+O=iC4H3+OH           1.512E7           1.91  3.74e+03
      !H_Abstraction exact:   Cd_pri     O_atom_triplet
      deltaHrxn(T=298K) = -13.32889325413017 kcal/mol
iC4H3+H2O2=C4H4-123+HO2 28.8        3.1         6.94e+03
      !H_Abstraction estimate: (Average:) Cd_pri_rad     H2O2
      deltaHrxn(T=298K) = -3.8694322217068517 kcal/mol
C4H4-123+O2=iC4H3+HO2   2.8672E14   0.0         60.01e+03
      !H_Abstraction exact:   Cd_pri     O2b          deltaHrxn(T=298K)
= 3.869434729610186 kcal/mol

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!Validated before these additions!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

C4H7OJ(9)+H2=C4H8O-enol+H     9.14E11     0.0   14.8e+03
      !H_Abstraction exact:   H2     C_rad/H2/Cs      deltaHrxn(T=298K)
= -8.591372559702067E-4 kcal/mol

!Replace high-p limit kinetics
C3H6O-enol2+O2=C3H5O-enol2+HO2      1.588E14    0.0   47.69e+03
      !H_Abstraction estimate: (Average:) C/H2/OneDeO     O2b
      deltaHrxn(T=298K) = -4.599751154855092 kcal/mol

C4H6-13+O=nC4H5+OH            1.512E7           1.91  3.74e+03
      !H_Abstraction exact:   Cd_pri     O_atom_triplet
      deltaHrxn(T=298K) = 8.86880364613206 kcal/mol
C4H6-13+O=iC4H5+OH            1.204E11    0.7         7.63e+03
      !H_Abstraction estimate: (Average:) Cd/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -2.5301122203407456 kcal/mol
C4H6-13+O2=nC4H5+HO2    2.8672E14   0.0         60.01e+03
      !H_Abstraction exact:   Cd_pri     O2b          deltaHrxn(T=298K)
= 26.067131629872417 kcal/mol
C4H6-13+O2=iC4H5+HO2    7.94E13           0.0         57.29e+03
      !H_Abstraction estimate: (Average:) No comment  Keq
=2.023337180238115      deltaHrxn(T=298K) = 59.743737417368315 kcal/mol
nC4H5+H2O2=C4H6-13+HO2  28.8        3.1         6.94e+03
      !H_Abstraction estimate: (Average:) Cd_pri_rad     H2O2
      deltaHrxn(T=298K) = -26.067129121969096 kcal/mol
iC4H5+H2O2=C4H6-13+HO2  28.8        3.1         6.94e+03
      !H_Abstraction estimate: (Average:) Cd_rad/OneDe     H2O2
      deltaHrxn(T=298K) = -14.66821325549629 kcal/mol

!September 8, 2010
!Following C3H5 PES from J.A. Miller et al.; J.Phys.Chem.A
H+aC3H4=aC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001316   2.21e+61    -15.25      20076 /
PLOG / 0.039474   1.24e+52    -12.02      17839 /
PLOG / 1          4.67e+51    -11.45      21340 /
PLOG / 10         3.75e+48    -10.27      22511 /
PLOG / 100        4.23e+43    -8.61 22522 /
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H+aC3H4=aC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001316         2.80e+38    -8.67 8035 /
PLOG / 0.039474         6.93e+36    -8.19 7462 /
PLOG / 1                3.32e+30    -5.78 6913 /
PLOG / 10               2.29e+26    -4.32 6163 /
PLOG / 100              4.38e+21    -2.71 5187 /

H+aC3H4=H+pC3H4   1.0   0.0   0.0
DUPLICATE
PLOG / 0.001316         8.49e+10    0.89  2503 /
PLOG / 0.039474         1.48e+13    0.26  4103 /
PLOG / 1                2.48e+15    -0.33 6436 /
PLOG / 10               2.35e+25    -3.23 13165 /
PLOG / 100              1.02e+24    -2.67 15552 /

H+aC3H4=H+pC3H4   1.0   0.0   0.0
DUPLICATE
PLOG / 10         1.74e+07    1.98  4521 /
PLOG / 100        4.63e+04    2.62  4466 /

H+aC3H4=CH3+C2H2  1.0   0.0   0.0
DUPLICATE
PLOG / 0.001316         1.23e+08    1.53  4737 /
PLOG / 0.039474         2.72e+09    1.20  6834 /
PLOG / 1                1.26e+20    -1.83 15003 /
PLOG / 10               1.68e+16    -0.60 14754 /
PLOG / 100              1.37e+17    -0.79 17603 /

H+aC3H4=CH3+C2H2  1.0   0.0   0.0
DUPLICATE
PLOG / 1    1.23E+04    2.68  6335 /
PLOG / 10   3.31E+08    1.14  8886 /
PLOG / 100  1.28E+06    1.71  9774 /

H+aC3H4=sC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      6.44E+102   -27.51      51768 /
PLOG / 0.039473684      1.55E+53    -13.1 14472 /
PLOG / 1    1.90E+53    -12.59      16726 /
PLOG / 10   7.95E+51    -11.82      18286 /
PLOG / 100  4.21E+52    -11.64      22262 /

H+aC3H4=sC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      1.10E+54    -14.29      10809 /
PLOG / 0.039473684      9.88E+44    -11.21      8212 /
PLOG / 1    2.81E+40    -9.42 7850 /
PLOG / 10   2.60E+35    -7.57 7147 /
PLOG / 100  9.88E+29    -5.53 6581 /

H+pC3H4=sC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      8.85E+51    -13.04      12325 /
PLOG / 0.039473684      3.17E+52    -12.69      14226 /
PLOG / 1    2.87E+53    -12.51      16853 /
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PLOG / 10   9.51E+51    -11.74      18331 /
PLOG / 100  4.51E+52    -11.58      22207 /

H+pC3H4=sC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      1.97E+46    -11.91      7456 /
PLOG / 0.039473684      2.59E+45    -11.23      8046 /
PLOG / 1    6.93E+39    -9.11 7458 /
PLOG / 10   6.80E+34    -7.29 6722 /
PLOG / 100  5.65E+29    -5.39 6150 /

H+pC3H4=pC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      -1.71E+39   -10.47      7722 /
PLOG / 0.039473684      3.38E+49    -12.75      14072 /
PLOG / 1    1.37E+51    -12.55      15428 /
PLOG / 10   3.88E+50    -11.9 16915 /
PLOG / 100  2.17E+49    -11.1 18746 /

H+pC3H4=pC3H5 1.0 0.0   0.0
DUPLICATE
PLOG / 0.001315789      1.49E+38    -10.11      7458 /
PLOG / 0.039473684      2.98E+43    -11.43      8736 /
PLOG / 1    5.75E+39    -9.51 8772 /
PLOG / 10   4.33E+40    -9.6  9401 /
PLOG / 100  3.44E+34    -7.36 8558 /

H+pC3H4=CH3+C2H2 1.0    0.0   0.0
DUPLICATE
PLOG / 0.001315789      2.44E+10    1.04  3980 /
PLOG / 0.039473684      3.89E+10    0.989 4114 /
PLOG / 1    3.46E+12    0.442 5463 /
PLOG / 10   1.72E+14    -0.01 7134 /
PLOG / 100  -7.41E+30   -5.54 12108 /

H+pC3H4=CH3+C2H2 1.0    0.0   0.0
DUPLICATE
PLOG / 100  1.90E+15    -0.29 8306 /

CH3+C2H2=pC3H5 1.0      0.0   0.0
DUPLICATE
PLOG / 0.001315789      -4.96E+126  -37.53      42751 /
PLOG / 0.039473684      -6.80E+48   -12.27      16642 /
PLOG / 1    1.19E+44    -10.19      18728 /
PLOG / 10   6.02E+43    -9.74 20561 /
PLOG / 100  1.42E+42    -8.91 22235 /

CH3+C2H2=pC3H5 1.0      0.0   0.0
DUPLICATE
PLOG / 0.001315789      1.78E+41    -10.4 13647 /
PLOG / 0.039473684      1.52E+44    -10.73      15256 /
PLOG / 1    8.49E+35    -8.43 12356 /
PLOG / 10   3.04E+32    -7.01 12357 /
PLOG / 100  1.69E+27    -5.07 11690 /

H+pC3H4=pC3H3+H2  3.57e+04    2.825 4821
H+aC3H4=pC3H3+H2  6.62e+03    3.095 5522
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!September 9, 2010
C4H8O-enol+H=C4H7O_1_2+H2     4.50e+04    2.67  3.48e+03     !Value from
C4H8-1+H=H2+C4H7-24

CHCHCHCHOH+H2=CH2CHCHCHOH+H   8.98E12     0.0   10.3e+03
      !H_Abstraction exact:   H2     Cd_pri_rad       deltaHrxn(T=298K)
= -6.989028104334074 kcal/mol
CH2CHCHCHOH+H=CH2CHCCHOH+H2   1.93E8      1.74  10.28e+03
      !H_Abstraction exact:   Cd/H/OneDe     H_rad
      deltaHrxn(T=298K) = -4.409887757794942 kcal/mol
CHCHCHCHOH+CH4=CH2CHCHCHOH+CH3      6.36E14     0.0   13.7e+03
      !H_Abstraction exact:   C_methane     Cd_pri_rad
      deltaHrxn(T=298K) = -6.319501836603589 kcal/mol
CH2CHCHCHOH+CH3=CH2CHCCHOH+CH4      5.78E13     0.0   16.2e+03
      !H_Abstraction exact:   Cd/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -5.079414025525427 kcal/mol
CH2CHCHCHOH+O=CHCHCHCHOH+OH   7560000.0   1.91  3.74e+03
      !H_Abstraction exact:   Cd_pri     O_atom_triplet
      deltaHrxn(T=298K) = 8.148909973240645 kcal/mol
CH2CHCHCHOH+O=CH2CHCCHOH+OH   6.020000000000009E10    0.7   7.63e+03
      !H_Abstraction estimate: (Average:) Cd/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -3.2500058888883707 kcal/mol
CH2CHCHCHOH+OH=CHCHCHCHOH+H2O 1.026E13    0.0   5.94e+03
      !H_Abstraction exact:   Cd_pri     O_pri_rad
      deltaHrxn(T=298K) = -8.049321649225497 kcal/mol
CH2CHCHCHOH+OH=CH2CHCCHOH+H2O 1109999.9999999998      2.0   1.45e+03
      !H_Abstraction estimate: (Average:) Cd/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -19.448237511354513 kcal/mol
CH2CHCHCHOH+O2=CHCHCHCHOH+HO2 1.4336E14   0.0   60.01e+03
      !H_Abstraction exact:   Cd_pri     O2b          deltaHrxn(T=298K)
= 61.48365777932816 kcal/mol
CH2CHCHCHOH+O2=CH2CHCCHOH+HO2 3.97E13           0.0   57.29e+03
      !H_Abstraction estimate: (Average:) No comment  Keq
=4.741378828662712E-6   deltaHrxn(T=298K) = 50.084741917199146 kcal/mol

!CH2CHCHCHOH(+m)=iC4H5+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit Reverse: R_Recombination
estimate: (Average:)Cd_pri_rad     O_pri_rad          deltaHrxn(T=298K)
= 109.90848338015522 kcal/mol
!TCHEB / 300.0 2000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 4   4 /
!CHEB / -3.0148000e+01 4.8962000e-01 -1.2319000e-01 1.7173000e-02 /
!CHEB / 3.3277000e+01 7.1390000e-01 -1.1264000e-01 -1.5904000e-02 /
!CHEB / -4.7979000e-01 3.8368000e-01 2.0007000e-03 -3.2767000e-02 /
!CHEB / -2.7489000e-01 1.5021000e-01 4.4588000e-02 -1.9695000e-02 /

!September 12, 2010
CHCCHCHOH+H=CHCCCHOH+H2       1.93E8      1.74  10.28e+03
      !H_Abstraction exact:   Cd/H/OneDe     H_rad
      deltaHrxn(T=298K) = -2.4600674293742784 kcal/mol
CHCCHCHOH+CH3=CHCCCHOH+CH4    5.78E13     0.0   16.2e+03
      !H_Abstraction exact:   Cd/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -3.1295936971047524 kcal/mol
CHCCHCHOH+OH=CHCCCHOH+H2O     1.11E6      2.0   1.45e+03
      !H_Abstraction estimate: (Average:) Cd/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -17.498417182933835 kcal/mol
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CHCCHCHOH+O=CHCCCHOH+OH       6.02E10     0.7   7.63e+03
      !H_Abstraction estimate: (Average:) Cd/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -1.3001855604676926 kcal/mol

!September 18, 2010
!Adding C3H4O H-abstractions
CHCHCHO+H2O2=C3H4O+HO2  28.8  3.1   6.94e+03    !H_Abstraction estimate:
(Average:)  Cd_pri_rad     H2O2           deltaHrxn(T=298K) = -
26.067129317394638 kcal/mol
tSPC(346)+H2O2=C3H4O+HO2      28.8  3.1   6.94e+03    !H_Abstraction
estimate: (Average:)    Cd_rad/OneDe     H2O2         deltaHrxn(T=298K)
= -14.66821325639966 kcal/mol
C3H4O+HO2=C3H3O-enone+H2O2    5.486E12    0.0   5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_rad/NonDeO
      deltaHrxn(T=298K) = -2.130025337753125 kcal/mol

C3H4O+O2=CHCHCHO+HO2    1.4336E14   0.0   60.01e+03   !H_Abstraction
exact:      Cd_pri     O2b          deltaHrxn(T=298K) =
26.067131825297963 kcal/mol
C3H4O+O2=tSPC(346)+HO2  3.97E13           0.0   63.03354957036987e+03
      !H_Abstraction estimate: (Average:) No comment  Keq
=4.1222882288763 85E-7   deltaHrxn(T=298K) = 63.03354957036987 kcal/mol
!C3H4O+O2=C3H3O-enone+HO2     1.204E14    0.0   39.15e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O2b
      deltaHrxn(T=298K) = -2.130022829849803 kcal/mol

C3H4O+O=CHCHCHO+OH      7560000.0   1.91  3.74e+03    !H_Abstraction
exact:      Cd_pri     O_atom_triplet           deltaHrxn(T=298K) =
8.86880384155761 kcal/mol
C3H4O+O=tSPC(346)+OH    6.02E10     0.7   7.63e+03    !H_Abstraction
estimate: (Average:)    Cd/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -2.530112219437365 kcal/mol
!C3H4O+O=C3H3O-enone+OH 5.00E12     0.0   1.79e+03    !H_Abstraction
estimate: (Average:)    CO/H/OneDe     O_atom_triplet
      deltaHrxn(T=298K) = -19.328350813590156 kcal/mol

C3H4O+OH=CHCHCHO+H2O    1.026E13    0.0   5.94e+03    !H_Abstraction
exact:      Cd_pri     O_pri_rad          deltaHrxn(T=298K) = -
8.01929550100737 kcal/mol
C3H4O+OH=tSPC(346)+H2O  1110000.0   2.0   1.45e+03    !H_Abstraction
estimate: (Average:)    Cd/H/OneDe     O_pri_rad      deltaHrxn(T=298K)
= -19.41821156200234 kcal/mol
!C3H4O+OH=C3H3O-enone+H2O     5.486E12    0.0   5.96e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     O_pri_rad
      deltaHrxn(T=298K) = -36.21645015615513 kcal/mol

CHCHCHO+H2=C3H4O+H      8.98E12     0.0   10.3e+03    !H_Abstraction
exact:      H2     Cd_pri_rad       deltaHrxn(T=298K) = -
10.099760481682267 kcal/mol
C3H4O+H=tSPC(346)+H2    1.93E8      1.74  10.28e+03   !H_Abstraction
exact:      Cd/H/OneDe     H_rad          deltaHrxn(T=298K) = -
1.299155579312707 kcal/mol
!C3H4O+H=C3H3O-enone+H2 8.07E7      1.76  0.67e+03    !H_Abstraction
estimate: (Average:)    CO/H/OneDe     H_rad          deltaHrxn(T=298K)
= -18.0973941734655 kcal/mol
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CHCHCHO+CH4=C3H4O+CH3   6.36E14     0.0   13.7e+03    !H_Abstraction
exact:      C_methane     Cd_pri_rad      deltaHrxn(T=298K) = -
6.389476196545807 kcal/mol
C3H4O+CH3=tSPC(346)+CH4 5.78E13     0.0   16.2e+03    !H_Abstraction
exact:      Cd/H/OneDe     C_methyl       deltaHrxn(T=298K) = -
5.009439864449167 kcal/mol
!C3H4O+CH3=C3H3O-enone+CH4    1.05338E8   1.145 6.325e+03
      !H_Abstraction estimate: (Average:) CO/H/OneDe     C_methyl
      deltaHrxn(T=298K) = -21.807678458601956 kcal/mol

!September 20, 2010
CHCHCHCHOH+H2O2=CH2CHCHCHOH+HO2     28.8  3.1   6.94e+03
      !H_Abstraction estimate: (Average:) Cd_pri_rad     H2O2
      deltaHrxn(T=298K) = -26.067129124777104 kcal/mol
CH2CHCCHOH+H2O2=CH2CHCHCHOH+HO2     28.8  3.1   6.94e+03
      !H_Abstraction estimate: (Average:) Cd_rad/OneDe     H2O2
      deltaHrxn(T=298K) = -14.668213262648088 kcal/mol
C4H7-14+H2O2=C4H8-1+HO2 2.0305      3.29  1.0725e+03  !H_Abstraction
exact:      H2O2     C_rad/H2/Cs          deltaHrxn(T=298K) = -
15.968227939149607 kcal/mol
C2H3+H2O2=C2H4+HO2      28.8  3.1   6.94e+03    !H_Abstraction estimate:
(Average:)  InChI=1/C2H3/c1-2/h1H,2H2     H2O2        deltaHrxn(T=298K)
= -26.067129196807223 kcal/mol
C4H9O-1+C4H6O3(21)=nC4H10O+C4H5O3J(1)     1.01525     3.29  1.0725e+03
      !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-2-3-4-
5/h5H,1-4H2     O/H/NonDeO          deltaHrxn(T=298K) = -
2.7695334765961377 kcal/mol
nC4H10O+C4H5O3J(1)=C4H9O-2+C4H6O3(21)     5.6E12      0.0   17.686e+03
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeO
      deltaHrxn(T=298K) = 0.11988628701273285 kcal/mol
nC4H10O+C4H5O3J(1)=C4H9O-3+C4H6O3(21)     5.6E12      0.0   17.686e+03
      !H_Abstraction exact:   C/H2/NonDeC     O_rad/NonDeO
      deltaHrxn(T=298K) = 0.11987512265957889 kcal/mol
nC4H10O+C4H5O3J(1)=C4H9O-4+C4H6O3(21)     7900000.0   1.9   0.16e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     O_rad/NonDeO
      deltaHrxn(T=298K) = -2.9401003368544423 kcal/mol
C4H9O-5+C4H6O3(21)=nC4H10O+C4H5O3J(1)     17.3  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeO
      deltaHrxn(T=298K) = -5.729271313746921 kcal/mol

C4H9O-1+C4H8O-enol3=nC4H10O+C4H7O-13      3.119999999999999E-4    4.31
      3.39e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H2/OneDeC          deltaHrxn(T=298K) = -
15.498316284750523 kcal/mol
C4H9O-2+C4H8O-enol3=nC4H10O+C4H7O-13      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -12.84866909516711 kcal/mol
C4H9O-3+C4H8O-enol3=nC4H10O+C4H7O-13      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -12.848657930813964 kcal/mol
C4H9O-4+C4H8O-enol3=nC4H10O+C4H7O-13      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -9.788682471299943 kcal/mol
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C4H9O-5+C4H8O-enol3=nC4H10O+C4H7O-13      7899999.9999999935      1.9
      0.16e+03    !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H2/OneDeC       deltaHrxn(T=298K) = -18.458054121901306 kcal/mol
C4H9O-1+C4H8O-enol2=nC4H10O+C4H7O-13      1.6800000000000015E12   0.0
      12.4e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H3/Cd       deltaHrxn(T=298K) = -
13.728479158585962 kcal/mol
C4H9O-2+C4H8O-enol2=nC4H10O+C4H7O-13      8.609999999999989E11    0.0
      12.3e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h2,5H,3-4H2,1H3     C/H3/Cd       deltaHrxn(T=298K) = -
11.07883196900255 kcal/mol
C4H9O-3+C4H8O-enol2=nC4H10O+C4H7O-13      8.609999999999989E11    0.0
      12.3e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h3,5H,2,4H2,1H3     C/H3/Cd       deltaHrxn(T=298K) = -
11.078820804649403 kcal/mol
C4H9O-4+C4H8O-enol2=nC4H10O+C4H7O-13      1.1723092595386273E-5   5.02
      3.6500000000000004e+03  !H_Abstraction estimate: (Average:)
      InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3     C/H3/Cd
      deltaHrxn(T=298K) = -8.018845345135382 kcal/mol
C4H9O-5+C4H8O-enol2=nC4H10O+C4H7O-13      0.005203142341343064    4.47
      5.1e+03     !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H3/Cd           deltaHrxn(T=298K) = -16.688216995736745 kcal/mol
C4H9O-1+C4H8O-enol3=nC4H10O+C4H7O-14      8.499999999999997E-6    5.01
      5.01e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H2/CsO      deltaHrxn(T=298K) = -
5.709633774102308 kcal/mol
C4H9O-2+C4H8O-enol3=nC4H10O+C4H7O-14      2.1200000000000013E-6   5.06
      4.89e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h2,5H,3-4H2,1H3     C/H2/CsO      deltaHrxn(T=298K) = -
3.059986584518896 kcal/mol
C4H9O-3+C4H8O-enol3=nC4H10O+C4H7O-14      2.1200000000000013E-6   5.06
      4.89e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h3,5H,2,4H2,1H3     C/H2/CsO      deltaHrxn(T=298K) = -
3.059975420165749 kcal/mol
nC4H10O+C4H7O-14=C4H9O-4+C4H8O-enol3      8.832666641507531E-5
      4.539999999999999 6.404999999999999e+03   !H_Abstraction estimate:
(Average:)  C/H2/CsO     C_rad/H/CsO      deltaHrxn(T=298K) = -
3.93482721960936E-8 kcal/mol
C4H9O-5+C4H8O-enol3=nC4H10O+C4H7O-14      7899999.9999999935      1.9
      0.16e+03    !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H2/CsO          deltaHrxn(T=298K) = -8.66937161125309 kcal/mol
C4H9O-1+C4H8O-enol=nC4H10O+C4H7O_1_2      3.119999999999999E-4    4.31
      3.39e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H2/OneDeC         deltaHrxn(T=298K) = -
15.49831626778193 kcal/mol
C4H9O-2+C4H8O-enol=nC4H10O+C4H7O_1_2      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -12.848669078198519 kcal/mol
C4H9O-3+C4H8O-enol=nC4H10O+C4H7O_1_2      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -12.848657913845372 kcal/mol
C4H9O-4+C4H8O-enol=nC4H10O+C4H7O_1_2      193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -9.78868245433135 kcal/mol
```

```
C4H9O-5+C4H8O-enol=nC4H10O+C4H7O_1_2      7899999.9999999935      1.9
      0.16e+03    !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H2/OneDeC       deltaHrxn(T=298K) = -18.458054104932714 kcal/mol
C4H9O-1+C4H8O-enol2=nC4H10O+C4H7O_1_2     3.119999999999999E-4    4.31
      3.39e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H2/OneDeO         deltaHrxn(T=298K) = -
20.057870161502102 kcal/mol
C4H9O-2+C4H8O-enol2=nC4H10O+C4H7O_1_2     193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3
C/H2/OneDeO       deltaHrxn(T=298K) = -17.40822297191869 kcal/mol
C4H9O-3+C4H8O-enol2=nC4H10O+C4H7O_1_2     193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3
C/H2/OneDeO       deltaHrxn(T=298K) = -17.408211807565543 kcal/mol
C4H9O-4+C4H8O-enol2=nC4H10O+C4H7O_1_2     193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3
C/H2/OneDeO       deltaHrxn(T=298K) = -14.348236348051522 kcal/mol
C4H9O-5+C4H8O-enol2=nC4H10O+C4H7O_1_2     7899999.9999999935      1.9
      0.16e+03    !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H2/OneDeO       deltaHrxn(T=298K) = -23.017607998652885 kcal/mol
nC4H10O+C4H7OJ(9)=C4H9O-1+C4H8O-enol      1977.0      2.71  12.92e+03
      !H_Abstraction exact:   C/H3/Cs     C_rad/H2/Cs
      deltaHrxn(T=298K) = 4.8656055184892466E-8 kcal/mol
nC4H10O+C4H7OJ(9)=C4H9O-2+C4H8O-enol      3080.0      2.66  10.1e+03
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
      deltaHrxn(T=298K) = -2.6496471409273568 kcal/mol
nC4H10O+C4H7OJ(9)=C4H9O-3+C4H8O-enol      3080.0      2.66  10.1e+03
      !H_Abstraction exact:   C/H2/NonDeC     C_rad/H2/Cs
      deltaHrxn(T=298K) = -2.6496583052804965 kcal/mol
nC4H10O+C4H7OJ(9)=C4H9O-4+C4H8O-enol      8.499999999999997E-6    5.01
      5.01e+03    !H_Abstraction exact:   C_rad/H2/Cs     C/H2/CsO
      deltaHrxn(T=298K) = -5.709633764794518 kcal/mol
C4H9O-5+C4H8O-enol=nC4H10O+C4H7OJ(9)      1.581E11    0.0   7.0e+03
      !H_Abstraction exact:   C/H3/Cs     O_rad/NonDeC
      deltaHrxn(T=298K) = -2.959737885806838 kcal/mol
C4H9O-1+nC4H8O=nC4H10O+C4H7OJ(12)   3.119999999999999E-4    4.31
      3.39e+03    !H_Abstraction estimate: (Average:) InChI=1/C4H9O/c1-
2-3-4-5/h5H,1-4H2     C/H2/OneDeC         deltaHrxn(T=298K) = -
5.909162003574153 kcal/mol
C4H9O-2+nC4H8O=nC4H10O+C4H7OJ(12)   193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -3.259514813990741 kcal/mol
C4H9O-3+nC4H8O=nC4H10O+C4H7OJ(12)   193.59160954264038
      2.9628571428571426      6.789285714285714e+03   !H_Abstraction
estimate: (Average:)    InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3
C/H2/OneDeC       deltaHrxn(T=298K) = -3.259503649637594 kcal/mol
nC4H10O+C4H7OJ(12)=C4H9O-4+nC4H8O   0.00368     4.02  7.92e+03
      !H_Abstraction estimate: (Average:) C/H2/CsO     C_rad/H/OneDeC
      deltaHrxn(T=298K) = 0.1995281901235728 kcal/mol
C4H9O-5+nC4H8O=nC4H10O+C4H7OJ(12)   7899999.9999999935      1.9
      0.16e+03    !H_Abstraction estimate: (Average:) O_rad/NonDeC
C/H2/OneDeC       deltaHrxn(T=298K) = -8.868899840724936 kcal/mol
C4H9O-1+C4H8O-enol=nC4H10O+C4H7OJ(12)     136.05773514200868
      2.700833333333333 6.460104166666667e+03   !H_Abstraction estimate:
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(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h5H,1-4H2     O/H/OneDe
      deltaHrxn(T=298K) = -13.098617254143363 kcal/mol
C4H9O-2+C4H8O-enol=nC4H10O+C4H7OJ(12)     136.05773514200868
      2.700833333333333 6.460104166666667e+03   !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3     O/H/OneDe
      deltaHrxn(T=298K) = -10.448970064559951 kcal/mol
C4H9O-3+C4H8O-enol=nC4H10O+C4H7OJ(12)     136.05773514200868
      2.700833333333333 6.460104166666667e+03   !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3     O/H/OneDe
      deltaHrxn(T=298K) = -10.448958900206804 kcal/mol
C4H9O-4+C4H8O-enol=nC4H10O+C4H7OJ(12)     136.05773514200868
      2.700833333333333 6.460104166666667e+03   !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3     O/H/OneDe
      deltaHrxn(T=298K) = -7.388983440692783 kcal/mol
C4H9O-5+C4H8O-enol=nC4H10O+C4H7OJ(12)     17.3  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/OneDe
      deltaHrxn(T=298K) = -16.058355091294146 kcal/mol

!September 20, 2010
CH3CHCHCHO+H=CH2CHCHCHO+H2    1299000.0   2.38  2.8e+03
      !H_Abstraction exact:   C/H3/Cd     H_rad       deltaHrxn(T=298K)
= -12.8978286091681 kcal/mol
CH3CHCHCHO+CH3=CH2CHCHCHO+CH4 241.20000000000002      2.92  7.16e+03
      !H_Abstraction exact:   C/H3/Cd     C_methyl
      deltaHrxn(T=298K) = -16.60811289430456 kcal/mol
CH3CHCHCHO+O=CH2CHCHCHO+OH    2850.0000000000005      3.05  3.123e+03
      !H_Abstraction estimate: (Average:) C/H3/Cd     O_atom_triplet
      deltaHrxn(T=298K) = -14.12878524929276 kcal/mol
CH3CHCHCHO+OH=CH2CHCHCHO+H2O  404.2136505652999 3.1979999999999995
      1.7759999999999998e+03  !H_Abstraction estimate: (Average:)
      C/H3/Cd     O_pri_rad         deltaHrxn(T=298K) = -
31.01688459185774 kcal/mol
CH2CHCHCHO+HO2=CH3CHCHCHO+O2  1.7499999999999977E10   0.0   -3.275e+03
      !H_Abstraction estimate: (Average:) C_rad/H2/Cd     Orad_O_H
      deltaHrxn(T=298K) = -3.069542734447595 kcal/mol
CH2CHCHCHO+H2O2=CH3CHCHCHO+HO2      2.0304986547865194
      3.2899999999999996      1.0725e+03  !H_Abstraction estimate:
(Average:)  C_rad/H2/Cd     H2O2          deltaHrxn(T=298K) = -
3.0695402265442695 kcal/mol

H2O2+C4H5O3J(1)=HO2+C4H6O3(21)      34.6  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) H2O2     O_rad/NonDeO
      deltaHrxn(T=298K) = -13.198694545028253 kcal/mol

C4H9O-1+C4H6O3(3)=nC4H10O+C4H5O3J(3)      1.0152493273932597
      3.2899999999999996      1.0725e+03  !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h5H,1-4H2     O/H/NonDeO
      deltaHrxn(T=298K) = -12.898513853987282 kcal/mol
C4H9O-2+C4H6O3(3)=nC4H10O+C4H5O3J(3)      0.92048907726487
      3.336666666666667 1.1383333333333332e+03  !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3     O/H/NonDeO
      deltaHrxn(T=298K) = -10.24886666440387 kcal/mol
C4H9O-3+C4H6O3(3)=nC4H10O+C4H5O3J(3)      0.92048907726487
      3.336666666666667 1.1383333333333332e+03  !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3     O/H/NonDeO
      deltaHrxn(T=298K) = -10.248855500050723 kcal/mol
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C4H9O-4+C4H6O3(3)=nC4H10O+C4H5O3J(3)      0.92048907726487
      3.336666666666667 1.1383333333333332e+03  !H_Abstraction estimate:
(Average:)  InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3     O/H/NonDeO
      deltaHrxn(T=298K) = -7.188880040536702 kcal/mol
C4H9O-5+C4H6O3(3)=nC4H10O+C4H5O3J(3)      17.3  3.4   -1.14e+03
      !H_Abstraction estimate: (Average:) O_rad/NonDeC     O/H/NonDeO
      deltaHrxn(T=298K) = -15.858251691138065 kcal/mol
H2O2+C4H5O3J(3)=HO2+C4H6O3(3) 34.6  3.4   -1.14e+03   !H_Abstraction
estimate: (Average:)    H2O2     O_rad/NonDeO         deltaHrxn(T=298K)
= -3.069714167637123 kcal/mol

aC3H5+HO2=OH+CH2CHCH2O  6.98e+10    0.5   -1967.13    !C.F Goldsmith
Proc. Combust. Inst.

O2+CH2CHCH2O=HO2+C3H4O  1.8066E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=268098.37480480794     deltaHrxn(T=298K) = -36.86624240246714 kcal/mol
H+CH2CHCH2O=H2+C3H4O    1.140117173637879E13    -0.071      -
0.002166666666666666e+03     !Disproportionation estimate: (Average:)
      No comment  Keq =2.812764742469823E12     deltaHrxn(T=298K) = -
91.36087207746122 kcal/mol
OH+CH2CHCH2O=H2O+C3H4O  1.140117173637879E13    -0.071      -
0.002166666666666666e+03     !Disproportionation estimate: (Average:)
      No comment  Keq =2.016288245722142E14     deltaHrxn(T=298K) = -
106.3992218310208 kcal/mol
O+CH2CHCH2O=OH+C3H4O    3.620000000000006E12    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=6.481569138041004E12   deltaHrxn(T=298K) = -90.20099020855466 kcal/mol
HO2+CH2CHCH2O=H2O2+C3H4O      1.140117173637879E13    -0.071      -
0.002166666666666666e+03     !Disproportionation estimate: (Average:)
      No comment  Keq =3.7393678794894757E9     deltaHrxn(T=298K) = -
74.87247417041536 kcal/mol
O2+C4H9Oi4=HO2+C4H8O-i3 1.8066E11   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=1654585.5929140472     deltaHrxn(T=298K) = -33.02654845245815 kcal/mol
H+C4H9Oi4=H2+C4H8O-i3   3.620E12    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=1.7359150433252576E13  deltaHrxn(T=298K) = -87.52117812745225 kcal/mol
OH+C4H9Oi4=H2O+C4H8O-i3 4.820E13    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=1.2443646795556652E15  deltaHrxn(T=298K) = -102.5595278810118 kcal/mol
O+C4H9Oi4=OH+C4H8O-i3   3.620E12    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=4.000140218338467E13   deltaHrxn(T=298K) = -86.36129625854568 kcal/mol
HO2+C4H9Oi4=H2O2+C4H8O-i3     4.820E13    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=2.3077738626776276E10  deltaHrxn(T=298K) = -71.03278022040638 kcal/mol
O+iC4H7OJ(15)=OH+C4H6Oi-13    9.04E13     0.0   0.0e+03
      !Disproportionation exact:    No comment  Keq
=2.302293019529602E11   deltaHrxn(T=298K) = -68.45320772164612 kcal/mol
O2+iC4H7OJ(48)=HO2+C4H6Oi-13  4.817600000000008E10    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=2112.973114313911      deltaHrxn(T=298K) = -22.74786975419716 kcal/mol
H+iC4H7OJ(48)=H2+C4H6Oi-13    3.5218932465779775E12   -0.071      -
0.002166666666666666e+03     !Disproportionation estimate: (Average:)
      No comment  Keq =2.216834131149016E10     deltaHrxn(T=298K) = -
77.24249942919126 kcal/mol
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OH+iC4H7OJ(48)=H2O+C4H6Oi-13  3.5218932465779775E12   -0.071      -
0.0021666666666666666e+03     !Disproportionation estimate: (Average:)
      No comment  Keq =1.5891043192707896E12    deltaHrxn(T=298K) = -
92.28084918275083 kcal/mol
O+iC4H7OJ(48)=OH+C4H6Oi-13    1.298092203987038E12    -
0.012278632478632479    0.9572152777777776e+03  !Disproportionation
estimate: (Average:)    No comment  Keq =5.108341793275804E10
      deltaHrxn(T=298K) = -76.08261756028469 kcal/mol
HO2+iC4H7OJ(48)=H2O2+C4H6Oi-13      3.5218932465779775E12   -0.071
      -0.0021666666666666666e+03    !Disproportionation estimate:
(Average:)  No comment  Keq =2.947121107930193E7      deltaHrxn(T=298K)
= -60.75410152214539 kcal/mol
O2+iC4H7OJ(51)=HO2+C4H6Oi-12  4.817600000000008E10    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=12.851408788945147     deltaHrxn(T=298K) = -5.113493232501696 kcal/mol
H+iC4H7OJ(51)=H2+C4H6Oi-12    9.040000000000015E11    0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=1.348310654957526E8    deltaHrxn(T=298K) = -59.60812290749578 kcal/mol
OH+iC4H7OJ(51)=H2O+C4H6Oi-12  1.2100000000000021E13   0.0   0.0e+03
      !Disproportionation estimate: (Average:)  No comment  Keq
=9.665162834719152E9    deltaHrxn(T=298K) = -74.64647266105536 kcal/mol
O+iC4H7OJ(51)=OH+C4H6Oi-12    1.298092203987038E12    -
0.012278632478632479    0.9572152777777776e+03  !Disproportionation
estimate: (Average:)    No comment  Keq =3.106967531877834E8
      deltaHrxn(T=298K) = -58.44824103858922 kcal/mol
HO2+iC4H7OJ(51)=H2O2+C4H6Oi-12      1.2100000000000021E13   0.0
      0.0e+03     !Disproportionation estimate: (Average:)  No comment
      Keq =179248.178085966   deltaHrxn(T=298K) = -43.11972500044992
kcal/mol

!C4H8O-i2=C4H8O-i3      8.59E+11    0.318 55900.00

!15-OCT-2010: Re-running every pressure-dependent network
!     Previous A+B(+m)=products(+m) were off by 6 orders of magnitude in
the forward direction
!     Since the reverse rate coefficient is calculated through
equilibrium, it too was off by 6 orders of magnitude

!PDepNetwork nC4H10O
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C4H9O-1           -16.27      88.99 26.95 32.82 38.15 42.65 49.68
      54.93 63.28  !MRH
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!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5             29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C2H5O-1          -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C4H9O-2          -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     C3H7-1           25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CH2OH            -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9O-3          -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H9-1           20.65 78.53 23.01 28.55 33.6  37.94 44.89 50.17
      58.56
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9O-4          -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     C4H9O-5          -13.43      82.96 26.61 32.68 38.16 42.84 50.26
      55.81 64.46  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     nC4H10O=C4H8-1+H2O      1.589e+03    2.80        61993.00
!     CH3+C3H7O-N1=nC4H10O    1.000e+13    0.00        0.00
!     C4H9O-1+H=nC4H10O       2.000e+14    0.00        0.00
!     C2H5+C2H5O-1=nC4H10O    1.000e+13    0.00        0.00
!     C4H9O-2+H=nC4H10O       2.000e+14    0.00        0.00
!     C3H7-1+CH2OH=nC4H10O    1.000e+13    0.00        0.00
!     C4H9O-3+H=nC4H10O       2.000e+14    0.00        0.00
!     C4H9-1+OH=nC4H10O       1.000e+13    0.00        0.00
!     C4H9O-4+H=nC4H10O       2.000e+14    0.00        0.00
!     C4H9O-5+H=nC4H10O       2.000e+14    0.00        0.00

nC4H10O(+m)=C4H8-1+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: ReactionLibrary: MRH-dehydration
      deltaHrxn(T=298K) = 9.508822029332165 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4583000e+01 1.9157000e-01 -2.0286000e-02 /
CHEB / 2.1744000e+01 3.6224000e-01 -3.6981000e-02 /
CHEB / -9.2302000e-02 3.0506000e-01 -2.7400000e-02 /
CHEB / -2.2319000e-01 2.2632000e-01 -1.4909000e-02 /
CHEB / -1.9941000e-01 1.4472000e-01 -3.2445000e-03 /

CH3+C3H7O-N1(+m)=nC4H10O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -90.3602774411286 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2518000e+01 3.7495000e-01 -3.6489000e-02 /
CHEB / -9.4407000e-01 6.7547000e-01 -5.8003000e-02 /
CHEB / -7.4974000e-01 4.8723000e-01 -2.3435000e-02 /
CHEB / -4.6140000e-01 2.6623000e-01 8.8051000e-03 /
CHEB / -2.5261000e-01 8.8732000e-02 2.2993000e-02 /
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CH3+C3H7O-N1(+m)=C4H8-1+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -80.85145541179642
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8282000e+00 -1.4962000e+00 -3.6500000e-02 /
CHEB / 3.1020000e+00 8.7387000e-01 -4.9148000e-02 /
CHEB / 4.6470000e-01 5.5149000e-01 1.1278000e-03 /
CHEB / -1.9363000e-01 2.1174000e-01 3.6913000e-02 /
CHEB / -2.2410000e-01 -1.0272000e-02 3.7497000e-02 /

C4H9O-1+H(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -101.90906048999024 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3664000e+01 4.7464000e-01 -4.9080000e-02 /
CHEB / -1.1753000e+00 8.1668000e-01 -6.5679000e-02 /
CHEB / -8.6386000e-01 5.1192000e-01 -3.4125000e-03 /
CHEB / -4.8253000e-01 2.0632000e-01 3.6914000e-02 /
CHEB / -2.1172000e-01 1.3782000e-02 3.7496000e-02 /

C4H9O-1+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -92.40023846065807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5971000e+00 -1.4172000e+00 -4.7611000e-02 /
CHEB / 2.5327000e+00 9.6303000e-01 -5.1028000e-02 /
CHEB / 3.0099000e-01 5.1940000e-01 2.4826000e-02 /
CHEB / -1.7650000e-01 1.2214000e-01 5.7017000e-02 /
CHEB / -1.5676000e-01 -7.3856000e-02 3.5663000e-02 /

C4H9O-1+H(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -11.548783048861642
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0924000e+01 -1.3197000e+00 -5.5008000e-02 /
CHEB / 2.7623000e+00 1.0575000e+00 -4.2251000e-02 /
CHEB / 3.7502000e-01 4.5263000e-01 5.3734000e-02 /
CHEB / -1.7897000e-01 5.2016000e-03 6.6342000e-02 /
CHEB / -1.2589000e-01 -1.3274000e-01 1.7600000e-02 /

C2H5+C2H5O-1(+m)=nC4H10O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -89.72069207914286 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2589000e+01 3.7011000e-01 -3.5981000e-02 /
CHEB / -1.0061000e+00 6.6792000e-01 -5.7524000e-02 /
CHEB / -7.5035000e-01 4.8448000e-01 -2.4027000e-02 /
CHEB / -4.7686000e-01 2.6781000e-01 7.6019000e-03 /
CHEB / -2.6475000e-01 9.2091000e-02 2.2059000e-02 /
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C2H5+C2H5O-1(+m)=C4H8-1+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -80.2118700498107
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8604000e+00 -1.4999000e+00 -3.6103000e-02 /
CHEB / 3.0630000e+00 8.6898000e-01 -4.8980000e-02 /
CHEB / 4.6751000e-01 5.5192000e-01 2.5889000e-04 /
CHEB / -2.1172000e-01 2.1567000e-01 3.5874000e-02 /
CHEB / -2.3849000e-01 -6.5418000e-03 3.7219000e-02 /

CH3+C3H7O-N1(+m)=C2H5+C2H5O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -0.639585361985727
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9409000e+00 -1.3886000e+00 -4.3777000e-02 /
CHEB / 3.8441000e+00 1.0030000e+00 -4.5829000e-02 /
CHEB / 3.5473000e-01 5.1537000e-01 2.9121000e-02 /
CHEB / -2.7505000e-01 8.5707000e-02 5.9053000e-02 /
CHEB / -1.9159000e-01 -1.0713000e-01 3.2229000e-02 /

C4H9O-1+H(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -12.18836841084737
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1574000e+01 -1.3224000e+00 -5.4655000e-02 /
CHEB / 2.4207000e+00 1.0555000e+00 -4.2503000e-02 /
CHEB / 2.9105000e-01 4.5526000e-01 5.2848000e-02 /
CHEB / -2.0752000e-01 8.3026000e-03 6.6263000e-02 /
CHEB / -1.3817000e-01 -1.3193000e-01 1.8276000e-02 /

C4H9O-2+H(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -98.47930410902632 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3782000e+01 4.3829000e-01 -4.3901000e-02 /
CHEB / -1.1549000e+00 7.6901000e-01 -6.3553000e-02 /
CHEB / -8.3161000e-01 5.1025000e-01 -1.2535000e-02 /
CHEB / -4.8779000e-01 2.3323000e-01 2.6349000e-02 /
CHEB / -2.3290000e-01 4.0913000e-02 3.3770000e-02 /

C4H9O-2+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -88.97048207969414
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5214000e+00 -1.4465000e+00 -4.2767000e-02 /
CHEB / 2.6512000e+00 9.3347000e-01 -5.0884000e-02 /
CHEB / 3.4740000e-01 5.3623000e-01 1.4871000e-02 /
CHEB / -1.9233000e-01 1.5581000e-01 5.0287000e-02 /
CHEB / -1.8363000e-01 -5.4299000e-02 3.8064000e-02 /
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C4H9O-2+H(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -8.119026667897712
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0590000e+01 -1.3449000e+00 -5.0159000e-02 /
CHEB / 3.1206000e+00 1.0411000e+00 -4.4244000e-02 /
CHEB / 4.0370000e-01 4.7784000e-01 4.4370000e-02 /
CHEB / -2.1042000e-01 3.1829000e-02 6.4946000e-02 /
CHEB / -1.4752000e-01 -1.2732000e-01 2.3633000e-02 /

C4H9O-1+H(+m)=C4H9O-2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -3.42975638096393
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2222000e+00 -1.2823000e+00 -6.0839000e-02 /
CHEB / 4.2347000e+00 1.0809000e+00 -3.8062000e-02 /
CHEB / 6.3718000e-01 4.1368000e-01 6.6239000e-02 /
CHEB / -8.9196000e-02 -3.3526000e-02 6.5886000e-02 /
CHEB / -7.7344000e-02 -1.3892000e-01 7.7858000e-03 /

C4H9O-2+H(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -8.758612029883441
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1248000e+01 -1.3477000e+00 -4.9804000e-02 /
CHEB / 2.7696000e+00 1.0387000e+00 -4.4420000e-02 /
CHEB / 3.2169000e-01 4.8037000e-01 4.3435000e-02 /
CHEB / -2.3878000e-01 3.5244000e-02 6.4704000e-02 /
CHEB / -1.6013000e-01 -1.2617000e-01 2.4262000e-02 /

C3H7-1+CH2OH(+m)=nC4H10O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -87.45098657728538 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2572000e+01 3.5135000e-01 -3.4067000e-02 /
CHEB / -9.1937000e-01 6.3813000e-01 -5.5617000e-02 /
CHEB / -7.1842000e-01 4.7257000e-01 -2.6035000e-02 /
CHEB / -4.6684000e-01 2.7259000e-01 3.1882000e-03 /
CHEB / -2.6648000e-01 1.0441000e-01 1.8423000e-02 /

C3H7-1+CH2OH(+m)=C4H8-1+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -77.94216454795321
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6840000e+00 -1.5144000e+00 -3.4644000e-02 /
CHEB / 3.2475000e+00 8.4960000e-01 -4.8304000e-02 /
CHEB / 5.1386000e-01 5.5260000e-01 -2.9027000e-03 /
CHEB / -2.1267000e-01 2.3028000e-01 3.1866000e-02 /
CHEB / -2.4993000e-01 8.2200000e-03 3.5868000e-02 /
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CH3+C3H7O-N1(+m)=C3H7-1+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -2.909290863843213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2372000e+00 -1.4001000e+00 -4.2492000e-02 /
CHEB / 3.5825000e+00 9.9143000e-01 -4.6089000e-02 /
CHEB / 3.7051000e-01 5.2330000e-01 2.5501000e-02 /
CHEB / -2.7642000e-01 1.0056000e-01 5.6989000e-02 /
CHEB / -1.9956000e-01 -9.9487000e-02 3.3893000e-02 /

C4H9O-1+H(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -14.458073912704856
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1759000e+01 -1.3328000e+00 -5.3392000e-02 /
CHEB / 2.2899000e+00 1.0474000e+00 -4.3428000e-02 /
CHEB / 2.7479000e-01 4.6498000e-01 4.9500000e-02 /
CHEB / -2.0942000e-01 2.0424000e-02 6.5836000e-02 /
CHEB / -1.4283000e-01 -1.2832000e-01 2.0789000e-02 /

C2H5+C2H5O-1(+m)=C3H7-1+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -2.269705501857486
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2177000e+00 -1.4031000e+00 -4.2131000e-02 /
CHEB / 3.5980000e+00 9.8828000e-01 -4.6128000e-02 /
CHEB / 3.6482000e-01 5.2535000e-01 2.4528000e-02 /
CHEB / -2.9743000e-01 1.0453000e-01 5.6390000e-02 /
CHEB / -2.1346000e-01 -9.7380000e-02 3.4296000e-02 /

C4H9O-2+H(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -11.028317531740926
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1465000e+01 -1.3584000e+00 -4.8533000e-02 /
CHEB / 2.6037000e+00 1.0294000e+00 -4.5066000e-02 /
CHEB / 3.1191000e-01 4.8963000e-01 3.9922000e-02 /
CHEB / -2.3960000e-01 4.8530000e-02 6.3652000e-02 /
CHEB / -1.6599000e-01 -1.2122000e-01 2.6562000e-02 /

C4H9O-3+H(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -99.67905766404826 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3820000e+01 4.4998000e-01 -4.5472000e-02 /
CHEB / -1.2166000e+00 7.8492000e-01 -6.4356000e-02 /
CHEB / -8.4287000e-01 5.1171000e-01 -9.8319000e-03 /
CHEB / -4.7839000e-01 2.2504000e-01 2.9777000e-02 /
CHEB / -2.2331000e-01 3.1961000e-02 3.5223000e-02 /
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C4H9O-3+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -90.1702356347161
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6255000e+00 -1.4372000e+00 -4.4203000e-02 /
CHEB / 2.5553000e+00 9.4342000e-01 -5.1035000e-02 /
CHEB / 3.3119000e-01 5.3143000e-01 1.7917000e-02 /
CHEB / -1.7912000e-01 1.4495000e-01 5.2579000e-02 /
CHEB / -1.7179000e-01 -6.1119000e-02 3.7505000e-02 /

C4H9O-3+H(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -9.318780222919662
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0784000e+01 -1.3369000e+00 -5.1590000e-02 /
CHEB / 2.9395000e+00 1.0468000e+00 -4.3737000e-02 /
CHEB / 3.9494000e-01 4.7008000e-01 4.7308000e-02 /
CHEB / -1.9168000e-01 2.2993000e-02 6.5562000e-02 /
CHEB / -1.3743000e-01 -1.2947000e-01 2.1781000e-02 /

C4H9O-1+H(+m)=C4H9O-3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -2.2300028259419733
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0878000e+00 -1.2749000e+00 -6.2213000e-02 /
CHEB / 4.4250000e+00 1.0844000e+00 -3.7010000e-02 /
CHEB / 6.5350000e-01 4.0564000e-01 6.8704000e-02 /
CHEB / -8.1109000e-02 -4.0076000e-02 6.5440000e-02 /
CHEB / -7.2197000e-02 -1.3915000e-01 5.8233000e-03 /

C4H9O-3+H(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -9.95836558490539
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1439000e+01 -1.3397000e+00 -5.1236000e-02 /
CHEB / 2.5919000e+00 1.0445000e+00 -4.3936000e-02 /
CHEB / 3.1217000e-01 4.7264000e-01 4.6386000e-02 /
CHEB / -2.2009000e-01 2.6311000e-02 6.5372000e-02 /
CHEB / -1.4993000e-01 -1.2843000e-01 2.2429000e-02 /

C4H9O-2+H(+m)=C4H9O-3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = 1.1997535550219496
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6133000e+00 -1.2988000e+00 -5.7484000e-02 /
CHEB / 4.9517000e+00 1.0730000e+00 -4.0293000e-02 /
CHEB / 6.3635000e-01 4.3149000e-01 6.0450000e-02 /
CHEB / -1.0873000e-01 -1.8794000e-02 6.6526000e-02 /
CHEB / -8.9816000e-02 -1.3821000e-01 1.2105000e-02 /
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C4H9O-3+H(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -12.228071086762876
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1645000e+01 -1.3503000e+00 -4.9967000e-02 /
CHEB / 2.4386000e+00 1.0356000e+00 -4.4668000e-02 /
CHEB / 2.9984000e-01 4.8208000e-01 4.2917000e-02 /
CHEB / -2.2122000e-01 3.9236000e-02 6.4521000e-02 /
CHEB / -1.5538000e-01 -1.2394000e-01 2.4811000e-02 /

C4H9-1+OH(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -95.42000187263196 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2503000e+01 4.1599000e-01 -4.1103000e-02 /
CHEB / -1.1014000e+00 7.3736000e-01 -6.1788000e-02 /
CHEB / -8.1069000e-01 5.0499000e-01 -1.7076000e-02 /
CHEB / -4.8966000e-01 2.4724000e-01 1.9885000e-02 /
CHEB / -2.4704000e-01 5.8184000e-02 3.0433000e-02 /

C4H9-1+OH(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -85.91117984329978
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1060000e+00 -1.4642000e+00 -4.0298000e-02 /
CHEB / 2.7777000e+00 9.1349000e-01 -5.0408000e-02 /
CHEB / 3.7900000e-01 5.4368000e-01 9.5041000e-03 /
CHEB / -2.0256000e-01 1.7625000e-01 4.5693000e-02 /
CHEB / -2.0333000e-01 -4.0022000e-02 3.8547000e-02 /

C4H9-1+OH(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -5.059724431503357
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9820000e+00 -1.3596000e+00 -4.7730000e-02 /
CHEB / 3.4357000e+00 1.0295000e+00 -4.4958000e-02 /
CHEB / 4.1468000e-01 4.9162000e-01 3.9011000e-02 /
CHEB / -2.3233000e-01 4.9180000e-02 6.3394000e-02 /
CHEB / -1.6378000e-01 -1.2212000e-01 2.6880000e-02 /

C4H9O-1+H(+m)=C4H9-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -6.489058617358285
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7219000e+00 -1.2959000e+00 -5.8499000e-02 /
CHEB / 3.3795000e+00 1.0734000e+00 -3.9781000e-02 /
CHEB / 4.6739000e-01 4.2833000e-01 6.1653000e-02 /
CHEB / -1.5049000e-01 -2.0410000e-02 6.6399000e-02 /
CHEB / -1.0581000e-01 -1.3771000e-01 1.1425000e-02 /
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C4H9-1+OH(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -5.6993097934890855
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6467000e+00 -1.3625000e+00 -4.7373000e-02 /
CHEB / 3.0770000e+00 1.0269000e+00 -4.5094000e-02 /
CHEB / 3.3460000e-01 4.9405000e-01 3.8057000e-02 /
CHEB / -2.6070000e-01 5.2769000e-02 6.3053000e-02 /
CHEB / -1.7659000e-01 -1.2074000e-01 2.7465000e-02 /

C4H9O-2+H(+m)=C4H9-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -3.0593022363943554
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3119000e+00 -1.3203000e+00 -5.3696000e-02 /
CHEB / 3.8267000e+00 1.0597000e+00 -4.2460000e-02 /
CHEB / 4.7397000e-01 4.5411000e-01 5.2809000e-02 /
CHEB / -1.8144000e-01 3.3733000e-03 6.6388000e-02 /
CHEB / -1.2487000e-01 -1.3493000e-01 1.7709000e-02 /

C4H9-1+OH(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -7.969015295346571
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8872000e+00 -1.3735000e+00 -4.6097000e-02 /
CHEB / 2.8833000e+00 1.0168000e+00 -4.5589000e-02 /
CHEB / 3.3124000e-01 5.0292000e-01 3.4482000e-02 /
CHEB / -2.6110000e-01 6.6687000e-02 6.1625000e-02 /
CHEB / -1.8328000e-01 -1.1488000e-01 2.9576000e-02 /

C4H9O-3+H(+m)=C4H9-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -4.259055791416305
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5324000e+00 -1.3126000e+00 -5.5113000e-02 /
CHEB / 3.6140000e+00 1.0645000e+00 -4.1740000e-02 /
CHEB / 4.7359000e-01 4.4611000e-01 5.5600000e-02 /
CHEB / -1.6312000e-01 -4.5660000e-03 6.6551000e-02 /
CHEB / -1.1561000e-01 -1.3618000e-01 1.5746000e-02 /

C4H9O-4+H(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -95.04982181464689 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3821000e+01 4.0531000e-01 -3.9844000e-02 /
CHEB / -1.0670000e+00 7.2168000e-01 -6.0860000e-02 /
CHEB / -7.8935000e-01 5.0136000e-01 -1.8970000e-02 /
CHEB / -4.8258000e-01 2.5309000e-01 1.6875000e-02 /
CHEB / -2.4463000e-01 6.6384000e-02 2.8622000e-02 /
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C4H9O-4+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -85.54099978531471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3527000e+00 -1.4725000e+00 -3.9227000e-02 /
CHEB / 2.8510000e+00 9.0352000e-01 -5.0117000e-02 /
CHEB / 4.0609000e-01 5.4645000e-01 7.1432000e-03 /
CHEB / -2.0000000e-01 1.8581000e-01 4.3431000e-02 /
CHEB / -2.0422000e-01 -3.2668000e-02 3.8509000e-02 /

C4H9O-4+H(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -4.68954437351829
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0126000e+01 -1.3665000e+00 -4.6695000e-02 /
CHEB / 3.6132000e+00 1.0236000e+00 -4.5213000e-02 /
CHEB / 4.2810000e-01 4.9770000e-01 3.6572000e-02 /
CHEB / -2.3571000e-01 5.7633000e-02 6.2502000e-02 /
CHEB / -1.6302000e-01 -1.1914000e-01 2.8288000e-02 /

C4H9O-4+H(+m)=C4H9O-1+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = 6.859238675343356
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2856000e+00 -1.3022000e+00 -5.7497000e-02 /
CHEB / 6.1474000e+00 1.0695000e+00 -4.0495000e-02 /
CHEB / 6.0044000e-01 4.3499000e-01 5.9524000e-02 /
CHEB / -1.0511000e-01 -1.3899000e-02 6.6500000e-02 /
CHEB / -8.9971000e-02 -1.3676000e-01 1.3103000e-02 /

C4H9O-4+H(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -5.329129735504019
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0794000e+01 -1.3694000e+00 -4.6337000e-02 /
CHEB / 3.2503000e+00 1.0210000e+00 -4.5331000e-02 /
CHEB / 3.4921000e-01 5.0008000e-01 3.5612000e-02 /
CHEB / -2.6415000e-01 6.1298000e-02 6.2115000e-02 /
CHEB / -1.7591000e-01 -1.1764000e-01 2.8848000e-02 /

C4H9O-4+H(+m)=C4H9O-2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = 3.4294822943794188
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1753000e+00 -1.3268000e+00 -5.2678000e-02 /
CHEB / 5.3872000e+00 1.0551000e+00 -4.2988000e-02 /
CHEB / 6.0462000e-01 4.6068000e-01 5.0525000e-02 /
CHEB / -1.3778000e-01 1.0650000e-02 6.6131000e-02 /
CHEB / -1.0811000e-01 -1.3333000e-01 1.9348000e-02 /
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C4H9O-4+H(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -7.598835237361504
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1047000e+01 -1.3805000e+00 -4.5058000e-02 /
CHEB / 3.0411000e+00 1.0104000e+00 -4.5760000e-02 /
CHEB / 3.4982000e-01 5.0873000e-01 3.2017000e-02 /
CHEB / -2.6453000e-01 7.5491000e-02 6.0514000e-02 /
CHEB / -1.8300000e-01 -1.1132000e-01 3.0854000e-02 /

C4H9O-4+H(+m)=C4H9O-3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = 4.6292358494013754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9972000e+00 -1.3191000e+00 -5.4100000e-02 /
CHEB / 5.6315000e+00 1.0601000e+00 -4.2326000e-02 /
CHEB / 6.0447000e-01 4.5272000e-01 5.3362000e-02 /
CHEB / -1.2725000e-01 2.4677000e-03 6.6412000e-02 /
CHEB / -1.0207000e-01 -1.3480000e-01 1.7405000e-02 /

C4H9O-4+H(+m)=C4H9-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = 0.3701800579850669
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7620000e+00 -1.3412000e+00 -5.0265000e-02 /
CHEB / 4.4243000e+00 1.0448000e+00 -4.3979000e-02 /
CHEB / 4.6747000e-01 4.7493000e-01 4.5323000e-02 /
CHEB / -2.0362000e-01 2.6820000e-02 6.5216000e-02 /
CHEB / -1.3839000e-01 -1.2952000e-01 2.2824000e-02 /

C4H9O-5+H(+m)=nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -104.74881800832169 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3721000e+01 5.0139000e-01 -5.3537000e-02 /
CHEB / -1.3245000e+00 8.4787000e-01 -6.6341000e-02 /
CHEB / -8.9034000e-01 5.0789000e-01 4.5508000e-03 /
CHEB / -4.9147000e-01 1.8467000e-01 4.4190000e-02 /
CHEB / -2.0701000e-01 -4.1993000e-03 3.8657000e-02 /

C4H9O-5+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -95.23999597898953
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7775000e+00 -1.3950000e+00 -5.1972000e-02 /
CHEB / 2.3248000e+00 9.8178000e-01 -5.0306000e-02 /
CHEB / 2.6609000e-01 5.0377000e-01 3.2917000e-02 /
CHEB / -1.7990000e-01 9.8209000e-02 6.1001000e-02 /
CHEB / -1.4996000e-01 -8.5016000e-02 3.2752000e-02 /
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C4H9O-5+H(+m)=CH3+C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -14.388540567193095
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1260000e+01 -1.3002000e+00 -5.9388000e-02 /
CHEB / 2.4183000e+00 1.0670000e+00 -3.9804000e-02 /
CHEB / 3.4542000e-01 4.3243000e-01 6.0888000e-02 /
CHEB / -1.7391000e-01 -1.2406000e-02 6.6315000e-02 /
CHEB / -1.2251000e-01 -1.3446000e-01 1.2791000e-02 /

C4H9O-5+H(+m)=C4H9O-1+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -2.839757518331453
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9092000e+00 -1.2407000e+00 -6.9662000e-02 /
CHEB / 4.3609000e+00 1.0954000e+00 -3.0627000e-02 /
CHEB / 6.8335000e-01 3.6826000e-01 7.9652000e-02 /
CHEB / -6.0312000e-02 -6.5405000e-02 6.1947000e-02 /
CHEB / -6.2183000e-02 -1.3719000e-01 -2.8978000e-03 /

C4H9O-5+H(+m)=C2H5+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -15.028125929178824
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1905000e+01 -1.3028000e+00 -5.9039000e-02 /
CHEB / 2.0821000e+00 1.0652000e+00 -4.0115000e-02 /
CHEB / 2.6060000e-01 4.3509000e-01 6.0051000e-02 /
CHEB / -2.0264000e-01 -9.5459000e-03 6.6349000e-02 /
CHEB / -1.3460000e-01 -1.3386000e-01 1.3481000e-02 /

C4H9O-5+H(+m)=C4H9O-2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -6.269513899295383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6277000e+00 -1.2636000e+00 -6.5134000e-02 /
CHEB / 3.8109000e+00 1.0873000e+00 -3.4789000e-02 /
CHEB / 6.2527000e-01 3.9350000e-01 7.2553000e-02 /
CHEB / -8.4013000e-02 -4.7822000e-02 6.4441000e-02 /
CHEB / -7.6531000e-02 -1.3830000e-01 3.0354000e-03 /

C4H9O-5+H(+m)=C3H7-1+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -17.29783143103631
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2071000e+01 -1.3130000e+00 -5.7785000e-02 /
CHEB / 1.9706000e+00 1.0581000e+00 -4.1264000e-02 /
CHEB / 2.4164000e-01 4.4500000e-01 5.6878000e-02 /
CHEB / -2.0533000e-01 1.6688000e-03 6.6363000e-02 /
CHEB / -1.3857000e-01 -1.3111000e-01 1.6069000e-02 /
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C4H9O-5+H(+m)=C4H9O-3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -5.069760344273426
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5070000e+00 -1.2564000e+00 -6.6478000e-02 /
CHEB / 3.9847000e+00 1.0902000e+00 -3.3585000e-02 /
CHEB / 6.4614000e-01 3.8556000e-01 7.4823000e-02 /
CHEB / -7.6460000e-02 -5.3756000e-02 6.3761000e-02 /
CHEB / -7.1765000e-02 -1.3819000e-01 1.1322000e-03 /

C4H9O-5+H(+m)=C4H9-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -9.328816135689738
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1018000e+00 -1.2769000e+00 -6.2837000e-02 /
CHEB / 2.9860000e+00 1.0809000e+00 -3.6802000e-02 /
CHEB / 4.4779000e-01 4.0804000e-01 6.8304000e-02 /
CHEB / -1.4479000e-01 -3.5890000e-02 6.5431000e-02 /
CHEB / -1.0415000e-01 -1.3782000e-01 6.6031000e-03 /

C4H9O-5+H(+m)=C4H9O-4+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nC4H10O)      deltaHrxn(T=298K) = -9.698996193674809
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8943000e+00 -1.2831000e+00 -6.1849000e-02 /
CHEB / 3.4267000e+00 1.0775000e+00 -3.7657000e-02 /
CHEB / 5.7883000e-01 4.1468000e-01 6.6321000e-02 /
CHEB / -9.7528000e-02 -2.9943000e-02 6.5771000e-02 /
CHEB / -8.7368000e-02 -1.3725000e-01 8.2664000e-03 /

!PDepNetwork sBuOH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sBuOH       -70.51      83.05 28.21 34.5  40.21 45.08 52.8  58.62
      67.9   !MRH
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HOCHC2H5    -17.02      78.74 21.22 25.67 29.69 33.11 38.51 42.57
      49.06
!     CH2CH[OH]C2H5     -20.29      85.12 28.32 34.19 39.3  43.58 50.27
      55.31 63.42  !MRH
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
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!     C4H9-2            18.01 78.98 21.99 27.3  32.36 36.82 44.06 49.58
      58.28
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3C[OH]C2H5      -28.11      85.48 27.09 32.67 37.82 42.25 49.33
      54.67 63.16  !MRH
!     CH3CH[OH]CH2      -14.14      76.56 22.67 26.97 30.74 33.91 38.93
      42.77 49.05
!     CH3CH[OH]CHCH3    -22.93      85.73 29.6  34.49 38.99 42.99 49.61
      54.76 63.12  !MRH
!     CH3CH[OH]CH2CH2   -21.44      85.19 28.95 34.38 39.34 43.58 50.3
      55.39 63.54  !MRH
!     CH3CH[O]C2H5      -16.68      81.26 27.15 33.15 38.5  43.06 50.3
      55.76 64.36  !MRH
!     C4H8-2      -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25 54.24
!Here are the path reactions and their high-P limit kinetics:
!     sBuOH=C4H8-1+H2O        6.181e+03    2.75        60687.00
!     CH3+HOCHC2H5=sBuOH      2.000e+13    0.00        0.00
!     CH2CH[OH]C2H5+H=sBuOH   1.000e+14    0.00        0.00
!     C2H5O-2+C2H5=sBuOH      2.000e+13    0.00        0.00
!     C4H9-2+OH=sBuOH         2.000e+13    0.00        0.00
!     CH3C[OH]C2H5+H=sBuOH    1.000e+14    0.00        0.00
!     CH3CH[OH]CH2+CH3=sBuOH  2.000e+13    0.00        0.00
!     CH3CH[OH]CHCH3+H=sBuOH  1.000e+14    0.00        0.00
!     CH3CH[OH]CH2CH2+H=sBuOH 1.000e+14    0.00        0.00
!     CH3CH[O]C2H5+H=sBuOH    1.000e+14    0.00        0.00
!     sBuOH=C4H8-2+H2O        6.030e+04    2.47        62194.10

sBuOH(+m)=C4H8-1+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: ReactionLibrary: MRH-dehydration
      deltaHrxn(T=298K) = 13.928503342644987 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3793000e+01 2.2464000e-01 -2.5903000e-02 /
CHEB / 2.1304000e+01 4.2272000e-01 -4.6963000e-02 /
CHEB / -1.7669000e-01 3.5052000e-01 -3.4146000e-02 /
CHEB / -2.7976000e-01 2.5233000e-01 -1.7707000e-02 /
CHEB / -2.3089000e-01 1.5268000e-01 -2.7405000e-03 /

CH3+HOCHC2H5(+m)=sBuOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -88.73070364261592 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2933000e+01 4.1013000e-01 -3.9275000e-02 /
CHEB / -1.2449000e+00 7.2997000e-01 -6.0285000e-02 /
CHEB / -8.3895000e-01 5.0624000e-01 -1.9403000e-02 /
CHEB / -5.1002000e-01 2.5441000e-01 1.6005000e-02 /
CHEB / -2.6228000e-01 6.5825000e-02 2.8266000e-02 /

CH3+HOCHC2H5(+m)=C4H8-1+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -74.80220029997093 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6766000e+00 -1.4621000e+00 -3.7269000e-02 /
CHEB / 2.7620000e+00 9.1659000e-01 -4.6832000e-02 /
CHEB / 3.5448000e-01 5.4383000e-01 8.5124000e-03 /
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CHEB / -2.3496000e-01 1.7387000e-01 4.2124000e-02 /
CHEB / -2.1515000e-01 -4.1954000e-02 3.5758000e-02 /

CH2CH[OH]C2H5+H(+m)=sBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -102.3089480177185 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3213000e+01 5.5657000e-01 -6.1189000e-02 /
CHEB / -1.3772000e+00 9.0112000e-01 -6.1206000e-02 /
CHEB / -9.5314000e-01 4.8807000e-01 2.1559000e-02 /
CHEB / -4.8070000e-01 1.3951000e-01 5.2539000e-02 /
CHEB / -1.7953000e-01 -3.2691000e-02 3.4583000e-02 /

CH2CH[OH]C2H5+H(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -88.38044467507352 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7170000e+00 -1.3372000e+00 -6.0214000e-02 /
CHEB / 2.2270000e+00 1.0204000e+00 -4.1375000e-02 /
CHEB / 1.9312000e-01 4.5669000e-01 5.0317000e-02 /
CHEB / -1.6002000e-01 4.1524000e-02 6.1151000e-02 /
CHEB / -1.1202000e-01 -1.0429000e-01 2.0131000e-02 /

CH2CH[OH]C2H5+H(+m)=CH3+HOCHC2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -13.578244375102585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1570000e+01 -1.2319000e+00 -7.0403000e-02 /
CHEB / 2.1254000e+00 1.0901000e+00 -2.4836000e-02 /
CHEB / 2.4082000e-01 3.5993000e-01 7.7655000e-02 /
CHEB / -1.4951000e-01 -6.4882000e-02 5.5946000e-02 /
CHEB / -8.5760000e-02 -1.3295000e-01 -4.2313000e-03 /

C2H5O-2+C2H5(+m)=sBuOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -87.01125488364092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2790000e+01 3.9988000e-01 -3.8338000e-02 /
CHEB / -1.1116000e+00 7.1475000e-01 -5.9718000e-02 /
CHEB / -8.3219000e-01 5.0252000e-01 -2.1240000e-02 /
CHEB / -5.2731000e-01 2.6003000e-01 1.3191000e-02 /
CHEB / -2.7814000e-01 7.3951000e-02 2.6542000e-02 /

C2H5O-2+C2H5(+m)=C4H8-1+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -73.08275154099593 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4546000e+00 -1.4705000e+00 -3.6372000e-02 /
CHEB / 2.9434000e+00 9.0662000e-01 -4.6657000e-02 /
CHEB / 3.6717000e-01 5.4662000e-01 6.3188000e-03 /
CHEB / -2.5823000e-01 1.8356000e-01 4.0089000e-02 /
CHEB / -2.3518000e-01 -3.4523000e-02 3.5841000e-02 /
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CH3+HOCHC2H5(+m)=C2H5O-2+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -1.7194487589750125 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0173000e+01 -1.3507000e+00 -4.5406000e-02 /
CHEB / 3.2004000e+00 1.0372000e+00 -4.1462000e-02 /
CHEB / 2.0480000e-01 4.8256000e-01 3.8945000e-02 /
CHEB / -3.0451000e-01 3.7110000e-02 5.9048000e-02 /
CHEB / -1.7697000e-01 -1.2500000e-01 2.2265000e-02 /

CH2CH[OH]C2H5+H(+m)=C2H5O-2+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -15.297693134077594
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2178000e+01 -1.2383000e+00 -6.9439000e-02 /
CHEB / 1.7423000e+00 1.0876000e+00 -2.5998000e-02 /
CHEB / 1.4519000e-01 3.6686000e-01 7.6017000e-02 /
CHEB / -1.8162000e-01 -5.9640000e-02 5.6692000e-02 /
CHEB / -9.9549000e-02 -1.3295000e-01 -2.7135000e-03 /

C4H9-2+OH(+m)=sBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -97.2000799351262 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2619000e+01 5.0054000e-01 -5.0389000e-02 /
CHEB / -1.3373000e+00 8.4861000e-01 -6.3563000e-02 /
CHEB / -9.4266000e-01 5.0943000e-01 3.1484000e-03 /
CHEB / -5.2764000e-01 1.8601000e-01 4.0986000e-02 /
CHEB / -2.2923000e-01 -2.5697000e-03 3.6518000e-02 /

C4H9-2+OH(+m)=C4H8-1+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -83.27157659248121 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9009000e+00 -1.3866000e+00 -4.8775000e-02 /
CHEB / 2.3730000e+00 9.9162000e-01 -4.6482000e-02 /
CHEB / 2.1571000e-01 4.9817000e-01 3.2900000e-02 /
CHEB / -2.1657000e-01 8.6784000e-02 5.7236000e-02 /
CHEB / -1.6313000e-01 -9.0570000e-02 2.8567000e-02 /

C4H9-2+OH(+m)=CH3+HOCHC2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -8.469376292510276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0478000e+01 -1.2773000e+00 -5.8643000e-02 /
CHEB / 2.5137000e+00 1.0819000e+00 -3.4663000e-02 /
CHEB / 2.4979000e-01 4.0684000e-01 6.4082000e-02 /
CHEB / -2.1729000e-01 -3.7041000e-02 6.0409000e-02 /
CHEB / -1.2805000e-01 -1.3679000e-01 5.3468000e-03 /

CH2CH[OH]C2H5+H(+m)=C4H9-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -5.108868082592309 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7487000e+00 -1.1710000e+00 -8.1928000e-02 /
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CHEB / 3.0897000e+00 1.1022000e+00 -1.1067000e-02 /
CHEB / 3.8394000e-01 2.9404000e-01 9.1877000e-02 /
CHEB / -1.0431000e-01 -1.0228000e-01 4.6325000e-02 /
CHEB / -5.8696000e-02 -1.2566000e-01 -1.7167000e-02 /

C4H9-2+OH(+m)=C2H5O-2+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -10.188825051485285 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1104000e+01 -1.2839000e+00 -5.7666000e-02 /
CHEB / 2.1115000e+00 1.0781000e+00 -3.5500000e-02 /
CHEB / 1.5738000e-01 4.1390000e-01 6.2083000e-02 /
CHEB / -2.4908000e-01 -3.0603000e-02 6.0718000e-02 /
CHEB / -1.4261000e-01 -1.3609000e-01 6.9734000e-03 /

CH3C[OH]C2H5+H(+m)=sBuOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -94.4898913884416 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3364000e+01 4.6092000e-01 -4.4753000e-02 /
CHEB / -1.2189000e+00 8.0065000e-01 -6.2706000e-02 /
CHEB / -8.9790000e-01 5.1456000e-01 -8.1597000e-03 /
CHEB / -5.1939000e-01 2.1905000e-01 3.0376000e-02 /
CHEB / -2.3852000e-01 2.5525000e-02 3.4677000e-02 /

CH3C[OH]C2H5+H(+m)=C4H8-1+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -80.56138804579662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4418000e+00 -1.4203000e+00 -4.2814000e-02 /
CHEB / 2.5976000e+00 9.6210000e-01 -4.7311000e-02 /
CHEB / 2.7263000e-01 5.2254000e-01 2.1175000e-02 /
CHEB / -2.2055000e-01 1.2431000e-01 5.1561000e-02 /
CHEB / -1.7730000e-01 -7.3371000e-02 3.3066000e-02 /

CH3C[OH]C2H5+H(+m)=CH3+HOCHC2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -5.759187745825685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0746000e+01 -1.3075000e+00 -5.2308000e-02 /
CHEB / 2.9970000e+00 1.0679000e+00 -3.8542000e-02 /
CHEB / 2.7946000e-01 4.3935000e-01 5.3741000e-02 /
CHEB / -2.3484000e-01 -1.0767000e-02 6.1308000e-02 /
CHEB / -1.3417000e-01 -1.3566000e-01 1.2471000e-02 /

CH2CH[OH]C2H5+H(+m)=CH3C[OH]C2H5+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -7.819056629276901
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2699000e+00 -1.1987000e+00 -7.6159000e-02 /
CHEB / 3.3247000e+00 1.0996000e+00 -1.8016000e-02 /
CHEB / 5.0878000e-01 3.2358000e-01 8.5819000e-02 /
CHEB / -6.0858000e-02 -8.8113000e-02 5.1201000e-02 /
CHEB / -4.5238000e-02 -1.3028000e-01 -1.1717000e-02 /
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CH3C[OH]C2H5+H(+m)=C2H5O-2+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -7.4786365048006935 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1391000e+01 -1.3142000e+00 -5.1339000e-02 /
CHEB / 2.5740000e+00 1.0633000e+00 -3.9140000e-02 /
CHEB / 1.9187000e-01 4.4629000e-01 5.1554000e-02 /
CHEB / -2.6662000e-01 -3.4172000e-03 6.1218000e-02 /
CHEB / -1.4948000e-01 -1.3424000e-01 1.4090000e-02 /

CH3C[OH]C2H5+H(+m)=C4H9-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = 2.7101885466845914 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5999000e+00 -1.2430000e+00 -6.4594000e-02 /
CHEB / 4.3445000e+00 1.0969000e+00 -2.9407000e-02 /
CHEB / 3.2070000e-01 3.6900000e-01 7.4344000e-02 /
CHEB / -1.7715000e-01 -6.6066000e-02 5.7543000e-02 /
CHEB / -9.7101000e-02 -1.3679000e-01 -2.9872000e-03 /

CH3CH[OH]CH2+CH3(+m)=sBuOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -91.61019936626036 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2847000e+01 4.3731000e-01 -4.2009000e-02 /
CHEB / -1.2614000e+00 7.6885000e-01 -6.1686000e-02 /
CHEB / -8.6878000e-01 5.1280000e-01 -1.3849000e-02 /
CHEB / -5.0023000e-01 2.3687000e-01 2.3668000e-02 /
CHEB / -2.4185000e-01 4.4031000e-02 3.2201000e-02 /

CH3CH[OH]CH2+CH3(+m)=C4H8-1+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -77.68169602361537 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7808000e+00 -1.4399000e+00 -3.9984000e-02 /
CHEB / 2.6347000e+00 9.4183000e-01 -4.7207000e-02 /
CHEB / 3.1118000e-01 5.3395000e-01 1.4913000e-02 /
CHEB / -2.1126000e-01 1.4750000e-01 4.7365000e-02 /
CHEB / -1.8590000e-01 -5.9979000e-02 3.4788000e-02 /

CH3CH[OH]CH2+CH3(+m)=CH3+HOCHC2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -2.8794957236444354
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8819000e+00 -1.3246000e+00 -4.9272000e-02 /
CHEB / 3.2386000e+00 1.0571000e+00 -3.9977000e-02 /
CHEB / 2.8903000e-01 4.5728000e-01 4.7760000e-02 /
CHEB / -2.3565000e-01 6.9741000e-03 6.0899000e-02 /
CHEB / -1.3750000e-01 -1.3290000e-01 1.6516000e-02 /

CH2CH[OH]C2H5+H(+m)=CH3CH[OH]CH2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -10.698748651458146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.0544000e+01 -1.2144000e+00 -7.3269000e-02 /
CHEB / 2.5670000e+00 1.0960000e+00 -2.1434000e-02 /
CHEB / 3.3635000e-01 3.4084000e-01 8.2031000e-02 /
CHEB / -1.1936000e-01 -7.7937000e-02 5.3627000e-02 /
CHEB / -7.0830000e-02 -1.3205000e-01 -8.2639000e-03 /

CH3CH[OH]CH2+CH3(+m)=C2H5O-2+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -4.598944482619448
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0540000e+01 -1.3315000e+00 -4.8309000e-02 /
CHEB / 2.7992000e+00 1.0520000e+00 -4.0447000e-02 /
CHEB / 2.0598000e-01 4.6406000e-01 4.5496000e-02 /
CHEB / -2.6773000e-01 1.4849000e-02 6.0555000e-02 /
CHEB / -1.5328000e-01 -1.3096000e-01 1.8088000e-02 /

C4H9-2+OH(+m)=CH3CH[OH]CH2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -5.589880568865837 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4027000e+00 -1.2593000e+00 -6.1580000e-02 /
CHEB / 3.0094000e+00 1.0907000e+00 -3.2121000e-02 /
CHEB / 3.3458000e-01 3.8713000e-01 6.9520000e-02 /
CHEB / -1.8726000e-01 -5.3244000e-02 5.9166000e-02 /
CHEB / -1.1108000e-01 -1.3748000e-01 9.2025000e-04 /

CH3C[OH]C2H5+H(+m)=CH3CH[OH]CH2+CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -2.8796920221812456
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6218000e+00 -1.2891000e+00 -5.5244000e-02 /
CHEB / 3.5508000e+00 1.0791000e+00 -3.6657000e-02 /
CHEB / 3.4902000e-01 4.1972000e-01 5.9764000e-02 /
CHEB / -2.0370000e-01 -2.9444000e-02 6.1085000e-02 /
CHEB / -1.1540000e-01 -1.3806000e-01 7.9665000e-03 /

CH3CH[OH]CHCH3+H(+m)=sBuOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -99.66896136778107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3499000e+01 5.1524000e-01 -5.2877000e-02 /
CHEB / -1.4936000e+00 8.6429000e-01 -6.3440000e-02 /
CHEB / -9.3814000e-01 5.0519000e-01 7.8037000e-03 /
CHEB / -4.9193000e-01 1.7346000e-01 4.4494000e-02 /
CHEB / -2.0202000e-01 -1.1641000e-02 3.6468000e-02 /

CH3CH[OH]CHCH3+H(+m)=C4H8-1+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -85.74045802513606 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8461000e+00 -1.3738000e+00 -5.1425000e-02 /
CHEB / 2.1845000e+00 1.0008000e+00 -4.5673000e-02 /
CHEB / 2.1661000e-01 4.8782000e-01 3.7484000e-02 /
CHEB / -1.7756000e-01 7.3835000e-02 5.8760000e-02 /
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CHEB / -1.3509000e-01 -9.5279000e-02 2.6508000e-02 /

CH3CH[OH]CHCH3+H(+m)=CH3+HOCHC2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -10.938257725165133
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1506000e+01 -1.2656000e+00 -6.1416000e-02 /
CHEB / 2.2501000e+00 1.0854000e+00 -3.2618000e-02 /
CHEB / 2.5630000e-01 3.9442000e-01 6.7853000e-02 /
CHEB / -1.7451000e-01 -4.5437000e-02 5.9566000e-02 /
CHEB / -1.0262000e-01 -1.3628000e-01 2.7199000e-03 /

CH2CH[OH]C2H5+H(+m)=CH3CH[OH]CHCH3+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -2.6399866499374482
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3465000e+00 -1.1605000e+00 -8.4370000e-02 /
CHEB / 4.0997000e+00 1.1018000e+00 -8.0476000e-03 /
CHEB / 6.2076000e-01 2.8320000e-01 9.3931000e-02 /
CHEB / -1.9863000e-02 -1.0654000e-01 4.4305000e-02 /
CHEB / -2.4461000e-02 -1.2357000e-01 -1.9013000e-02 /

CH3CH[OH]CHCH3+H(+m)=C2H5O-2+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -12.657706484140146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2127000e+01 -1.2722000e+00 -6.0439000e-02 /
CHEB / 1.8538000e+00 1.0820000e+00 -3.3545000e-02 /
CHEB / 1.6274000e-01 4.0147000e-01 6.5940000e-02 /
CHEB / -2.0637000e-01 -3.9331000e-02 6.0006000e-02 /
CHEB / -1.1694000e-01 -1.3580000e-01 4.3291000e-03 /

CH3CH[OH]CHCH3+H(+m)=C4H9-2+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -2.4688814326548574 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5689000e+00 -1.2032000e+00 -7.3424000e-02 /
CHEB / 3.3467000e+00 1.1042000e+00 -2.0617000e-02 /
CHEB / 3.6854000e-01 3.2573000e-01 8.5058000e-02 /
CHEB / -1.2663000e-01 -8.9879000e-02 5.1918000e-02 /
CHEB / -7.1545000e-02 -1.3159000e-01 -1.1585000e-02 /

CH3CH[OH]CHCH3+H(+m)=CH3C[OH]C2H5+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -5.179069979339452
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1413000e+00 -1.2316000e+00 -6.7338000e-02 /
CHEB / 3.5212000e+00 1.0989000e+00 -2.6914000e-02 /
CHEB / 5.0943000e-01 3.5684000e-01 7.7596000e-02 /
CHEB / -8.5546000e-02 -7.2829000e-02 5.6118000e-02 /
CHEB / -5.9522000e-02 -1.3541000e-01 -5.4339000e-03 /
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CH3CH[OH]CHCH3+H(+m)=CH3CH[OH]CH2+CH3(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -8.058762001520698
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0446000e+01 -1.2478000e+00 -6.4346000e-02 /
CHEB / 2.7289000e+00 1.0934000e+00 -2.9833000e-02 /
CHEB / 3.4486000e-01 3.7479000e-01 7.3031000e-02 /
CHEB / -1.4455000e-01 -6.0758000e-02 5.7994000e-02 /
CHEB / -8.6261000e-02 -1.3646000e-01 -1.6287000e-03 /

CH3CH[OH]CH2CH2+H(+m)=sBuOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -101.1589410829671 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3252000e+01 5.3914000e-01 -5.7443000e-02 /
CHEB / -1.3616000e+00 8.8695000e-01 -6.2526000e-02 /
CHEB / -9.4739000e-01 4.9609000e-01 1.5696000e-02 /
CHEB / -4.8658000e-01 1.5345000e-01 4.9499000e-02 /
CHEB / -1.8858000e-01 -2.4615000e-02 3.5653000e-02 /

CH3CH[OH]CH2CH2+H(+m)=C4H8-1+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -87.23043774032212
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6941000e+00 -1.3528000e+00 -5.6270000e-02 /
CHEB / 2.2711000e+00 1.0133000e+00 -4.3580000e-02 /
CHEB / 2.0220000e-01 4.7006000e-01 4.4972000e-02 /
CHEB / -1.6809000e-01 5.4358000e-02 6.0482000e-02 /
CHEB / -1.2105000e-01 -1.0119000e-01 2.2886000e-02 /

CH3CH[OH]CH2CH2+H(+m)=CH3+HOCHC2H5(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -12.428237440351182
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1472000e+01 -1.2463000e+00 -6.6411000e-02 /
CHEB / 2.2330000e+00 1.0891000e+00 -2.8488000e-02 /
CHEB / 2.4763000e-01 3.7429000e-01 7.3705000e-02 /
CHEB / -1.6021000e-01 -5.7421000e-02 5.7671000e-02 /
CHEB / -9.2377000e-02 -1.3463000e-01 -1.4007000e-03 /

CH2CH[OH]C2H5+H(+m)=CH3CH[OH]CH2CH2+H(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -1.1500069347514028
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7044000e+00 -1.1429000e+00 -8.8677000e-02 /
CHEB / 4.4923000e+00 1.0997000e+00 -2.5933000e-03 /
CHEB / 6.7268000e-01 2.6606000e-01 9.6934000e-02 /
CHEB / 2.3451000e-03 -1.1233000e-01 4.0858000e-02 /
CHEB / -1.4610000e-02 -1.1995000e-01 -2.1753000e-02 /
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CH3CH[OH]CH2CH2+H(+m)=C2H5O-2+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -14.147686199326191
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2086000e+01 -1.2528000e+00 -6.5437000e-02 /
CHEB / 1.8450000e+00 1.0862000e+00 -2.9556000e-02 /
CHEB / 1.5271000e-01 3.8129000e-01 7.1947000e-02 /
CHEB / -1.9221000e-01 -5.1830000e-02 5.8301000e-02 /
CHEB / -1.0637000e-01 -1.3445000e-01 1.6198000e-04 /

CH3CH[OH]CH2CH2+H(+m)=C4H9-2+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -3.9588611478409064 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6062000e+00 -1.1847000e+00 -7.8171000e-02 /
CHEB / 3.2477000e+00 1.1039000e+00 -1.5399000e-02 /
CHEB / 3.7977000e-01 3.0710000e-01 8.9200000e-02 /
CHEB / -1.1426000e-01 -9.7630000e-02 4.8776000e-02 /
CHEB / -6.3726000e-02 -1.2827000e-01 -1.4943000e-02 /

CH3CH[OH]CH2CH2+H(+m)=CH3C[OH]C2H5+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -6.669049694525498
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1473000e+00 -1.2127000e+00 -7.2254000e-02 /
CHEB / 3.4596000e+00 1.1002000e+00 -2.2106000e-02 /
CHEB / 5.1043000e-01 3.3734000e-01 8.2549000e-02 /
CHEB / -7.1565000e-02 -8.2320000e-02 5.3413000e-02 /
CHEB / -5.0861000e-02 -1.3262000e-01 -9.1906000e-03 /

CH3CH[OH]CH2CH2+H(+m)=CH3CH[OH]CH2+CH3(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -
9.548741716706743 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0433000e+01 -1.2287000e+00 -6.9312000e-02 /
CHEB / 2.6887000e+00 1.0958000e+00 -2.5330000e-02 /
CHEB / 3.4076000e-01 3.5493000e-01 7.8428000e-02 /
CHEB / -1.3018000e-01 -7.1387000e-02 5.5635000e-02 /
CHEB / -7.6905000e-02 -1.3413000e-01 -5.5804000e-03 /

CH3CH[OH]CH2CH2+H(+m)=CH3CH[OH]CHCH3+H(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -
1.4899797151860454 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1968000e+00 -1.1740000e+00 -8.0693000e-02 /
CHEB / 4.2663000e+00 1.1039000e+00 -1.2430000e-02 /
CHEB / 6.1418000e-01 2.9598000e-01 9.1473000e-02 /
CHEB / -2.9366000e-02 -1.0226000e-01 4.6813000e-02 /
CHEB / -2.9347000e-02 -1.2625000e-01 -1.6907000e-02 /

CH3CH[O]C2H5+H(+m)=sBuOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -105.91874789647454 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3367000e+01 6.0705000e-01 -7.3884000e-02 /
CHEB / -1.6530000e+00 9.3072000e-01 -5.3948000e-02 /
CHEB / -9.7503000e-01 4.6099000e-01 3.7988000e-02 /
CHEB / -4.8397000e-01 1.0368000e-01 5.8396000e-02 /
CHEB / -1.7258000e-01 -5.0202000e-02 3.0009000e-02 /

CH3CH[O]C2H5+H(+m)=C4H8-1+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -91.99024455382956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0020000e+01 -1.2915000e+00 -7.3318000e-02 /
CHEB / 1.8859000e+00 1.0317000e+00 -3.1649000e-02 /
CHEB / 1.6293000e-01 4.1823000e-01 6.4368000e-02 /
CHEB / -1.5978000e-01 1.0985000e-02 6.0675000e-02 /
CHEB / -1.0629000e-01 -1.0895000e-01 1.2232000e-02 /

CH3CH[O]C2H5+H(+m)=CH3+HOCHC2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -17.188044253858617 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2048000e+01 -1.1894000e+00 -8.3267000e-02 /
CHEB / 1.6422000e+00 1.0856000e+00 -1.1493000e-02 /
CHEB / 2.1159000e-01 3.2129000e-01 8.7108000e-02 /
CHEB / -1.4466000e-01 -8.1109000e-02 4.9878000e-02 /
CHEB / -8.5592000e-02 -1.2684000e-01 -1.1359000e-02 /

CH3CH[O]C2H5+H(+m)=CH2CH[OH]C2H5+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -3.6097998787560286
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0100000e+00 -1.0919000e+00 -1.0274000e-01 /
CHEB / 4.0072000e+00 1.0835000e+00 1.6269000e-02 /
CHEB / 6.9071000e-01 2.2305000e-01 1.0256000e-01 /
CHEB / 1.0158000e-02 -1.2227000e-01 3.0807000e-02 /
CHEB / -1.6136000e-02 -1.0938000e-01 -2.7640000e-02 /

CH3CH[O]C2H5+H(+m)=C2H5O-2+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -18.90749301283363 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2645000e+01 -1.1956000e+00 -8.2355000e-02 /
CHEB / 1.2700000e+00 1.0839000e+00 -1.2868000e-02 /
CHEB / 1.1480000e-01 3.2792000e-01 8.5827000e-02 /
CHEB / -1.7701000e-01 -7.6736000e-02 5.0870000e-02 /
CHEB / -9.8957000e-02 -1.2720000e-01 -1.0000000e-02 /

CH3CH[O]C2H5+H(+m)=C4H9-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -8.718667961348341 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3298000e+00 -1.1308000e+00 -9.3844000e-02 /
CHEB / 2.4950000e+00 1.0910000e+00 3.6106000e-03 /
CHEB / 3.7490000e-01 2.5968000e-01 9.7752000e-02 /
CHEB / -9.9901000e-02 -1.1172000e-01 3.8913000e-02 /
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CHEB / -6.2152000e-02 -1.1785000e-01 -2.2471000e-02 /

CH3CH[O]C2H5+H(+m)=CH3C[OH]C2H5+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -11.42885650803293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8052000e+00 -1.1573000e+00 -8.8622000e-02 /
CHEB / 2.7817000e+00 1.0910000e+00 -3.7506000e-03 /
CHEB / 4.8864000e-01 2.8705000e-01 9.3327000e-02 /
CHEB / -5.5511000e-02 -1.0026000e-01 4.4179000e-02 /
CHEB / -4.7230000e-02 -1.2290000e-01 -1.7887000e-02 /

CH3CH[O]C2H5+H(+m)=CH3CH[OH]CH2+CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -14.308548530214182
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1052000e+01 -1.1725000e+00 -8.5952000e-02 /
CHEB / 2.0530000e+00 1.0892000e+00 -7.5619000e-03 /
CHEB / 3.1126000e-01 3.0322000e-01 9.0476000e-02 /
CHEB / -1.1405000e-01 -9.1920000e-02 4.6990000e-02 /
CHEB / -7.1822000e-02 -1.2515000e-01 -1.4911000e-02 /

CH3CH[O]C2H5+H(+m)=CH3CH[OH]CHCH3+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -6.249786528693484
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9444000e+00 -1.1207000e+00 -9.6016000e-02 /
CHEB / 3.4854000e+00 1.0899000e+00 6.6747000e-03 /
CHEB / 6.1653000e-01 2.4970000e-01 9.9211000e-02 /
CHEB / -1.6149000e-02 -1.1512000e-01 3.6830000e-02 /
CHEB / -2.8335000e-02 -1.1570000e-01 -2.3992000e-02 /

CH3CH[O]C2H5+H(+m)=CH3CH[OH]CH2CH2+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -4.759806813507431
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3287000e+00 -1.1041000e+00 -9.9801000e-02 /
CHEB / 3.8466000e+00 1.0868000e+00 1.2049000e-02 /
CHEB / 6.7674000e-01 2.3398000e-01 1.0130000e-01 /
CHEB / 4.5947000e-03 -1.1966000e-01 3.3359000e-02 /
CHEB / -1.8985000e-02 -1.1207000e-01 -2.6218000e-02 /

sBuOH(+m)=C4H8-2+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH) High-P Limit: ReactionLibrary: MRH-dehydration
      deltaHrxn(T=298K) = 11.208700157174931 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4077000e+01 2.3050000e-01 -2.6309000e-02 /
CHEB / 2.1563000e+01 4.3320000e-01 -4.7578000e-02 /
CHEB / -2.2254000e-01 3.5780000e-01 -3.4284000e-02 /
CHEB / -2.9931000e-01 2.5561000e-01 -1.7349000e-02 /
CHEB / -2.3881000e-01 1.5249000e-01 -2.0974000e-03 /
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C4H8-2+H2O(+m)=C4H8-1+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = 2.719803185470056 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8642000e+01 -1.6061000e+00 -2.7954000e-02 /
CHEB / 2.4499000e+01 7.1416000e-01 -4.4835000e-02 /
CHEB / 1.3272000e+00 5.2471000e-01 -1.8535000e-02 /
CHEB / -9.8024000e-02 2.9432000e-01 7.5611000e-03 /
CHEB / -2.8660000e-01 9.9697000e-02 2.0865000e-02 /

CH3+HOCHC2H5(+m)=C4H8-2+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -77.52200348544099 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6989000e+00 -1.4585000e+00 -3.7357000e-02 /
CHEB / 2.7067000e+00 9.2126000e-01 -4.6588000e-02 /
CHEB / 3.4193000e-01 5.4323000e-01 9.3427000e-03 /
CHEB / -2.4064000e-01 1.6996000e-01 4.2776000e-02 /
CHEB / -2.1576000e-01 -4.5495000e-02 3.5637000e-02 /

CH2CH[OH]C2H5+H(+m)=C4H8-2+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -91.10024786054358 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7658000e+00 -1.3341000e+00 -6.0347000e-02 /
CHEB / 2.1524000e+00 1.0233000e+00 -4.0892000e-02 /
CHEB / 1.7970000e-01 4.5459000e-01 5.1126000e-02 /
CHEB / -1.6391000e-01 3.8089000e-02 6.1197000e-02 /
CHEB / -1.1266000e-01 -1.0601000e-01 1.9488000e-02 /

C2H5O-2+C2H5(+m)=C4H8-2+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -75.80255472646598 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4740000e+00 -1.4668000e+00 -3.6460000e-02 /
CHEB / 2.8905000e+00 9.1143000e-01 -4.6426000e-02 /
CHEB / 3.5464000e-01 5.4619000e-01 7.1386000e-03 /
CHEB / -2.6420000e-01 1.7967000e-01 4.0773000e-02 /
CHEB / -2.3584000e-01 -3.8187000e-02 3.5778000e-02 /

C4H9-2+OH(+m)=C4H8-2+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -85.99137977795127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9423000e+00 -1.3833000e+00 -4.8888000e-02 /
CHEB / 2.3033000e+00 9.9510000e-01 -4.6107000e-02 /
CHEB / 2.0265000e-01 4.9646000e-01 3.3767000e-02 /
CHEB / -2.2078000e-01 8.3002000e-02 5.7530000e-02 /
CHEB / -1.6366000e-01 -9.2921000e-02 2.8045000e-02 /

CH3C[OH]C2H5+H(+m)=C4H8-2+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -83.28119123126667 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4761000e+00 -1.4168000e+00 -4.2912000e-02 /
CHEB / 2.5329000e+00 9.6608000e-01 -4.7000000e-02 /
CHEB / 2.5982000e-01 5.2125000e-01 2.2043000e-02 /
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CHEB / -2.2522000e-01 1.2038000e-01 5.2028000e-02 /
CHEB / -1.7780000e-01 -7.6244000e-02 3.2691000e-02 /

CH3CH[OH]CH2+CH3(+m)=C4H8-2+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -80.40149920908543 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8101000e+00 -1.4364000e+00 -4.0077000e-02 /
CHEB / 2.5740000e+00 9.4612000e-01 -4.6928000e-02 /
CHEB / 2.9850000e-01 5.3297000e-01 1.5768000e-02 /
CHEB / -2.1633000e-01 1.4355000e-01 4.7923000e-02 /
CHEB / -1.8642000e-01 -6.3170000e-02 3.4523000e-02 /

CH3CH[OH]CHCH3+H(+m)=C4H8-2+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -88.46026121060612 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8897000e+00 -1.3706000e+00 -5.1543000e-02 /
CHEB / 2.1133000e+00 1.0041000e+00 -4.5270000e-02 /
CHEB / 2.0345000e-01 4.8599000e-01 3.8343000e-02 /
CHEB / -1.8166000e-01 7.0133000e-02 5.8988000e-02 /
CHEB / -1.3564000e-01 -9.7449000e-02 2.5944000e-02 /

CH3CH[OH]CH2CH2+H(+m)=C4H8-2+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sBuOH)   deltaHrxn(T=298K) = -89.95024092579217
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7409000e+00 -1.3496000e+00 -5.6397000e-02 /
CHEB / 2.1978000e+00 1.0163000e+00 -4.3131000e-02 /
CHEB / 1.8888000e-01 4.6805000e-01 4.5806000e-02 /
CHEB / -1.7205000e-01 5.0805000e-02 6.0603000e-02 /
CHEB / -1.2166000e-01 -1.0309000e-01 2.2270000e-02 /

CH3CH[O]C2H5+H(+m)=C4H8-2+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sBuOH)  deltaHrxn(T=298K) = -94.7100477392996 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0074000e+01 -1.2885000e+00 -7.3458000e-02 /
CHEB / 1.8083000e+00 1.0340000e+00 -3.1071000e-02 /
CHEB / 1.4920000e-01 4.1596000e-01 6.5081000e-02 /
CHEB / -1.6358000e-01 7.9011000e-03 6.0531000e-02 /
CHEB / -1.0705000e-01 -1.1024000e-01 1.1551000e-02 /

!PDepNetwork iBuOH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iBuOH       -68.34      83.38 27.21 33.74 39.68 44.72 52.64 58.55
      67.9   !MRH
!     iC4H8       -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34 54.27
!     H2O              -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH3              35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
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!     C3H7O-N2    -13.23      80.42 21.04 25.11 28.98 32.38 37.87 42.05
      48.76
!     C4H9Oi1     -18.28      86.11 28.03 33.68 38.81 43.16 49.99 55.12
      63.33  !MRH
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2           26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     CH2OH            -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9Oi2     -22.94      84.64 27.11 32.27 37.18 41.54 48.7  54.18
      62.91  !MRH
!     iC4H9       19.15 76.39 23.23 28.98 34.04 38.33 45.13 50.31 58.58
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9Oi3     -24.24      84.93 27.12 33.12 38.42 42.88 49.87 55.11
      63.43  !MRH
!     C4H9Oi4     -15.78      80.19 26.32 32.81 38.45 43.15 50.5  55.97
      64.52  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     iBuOH=iC4H8+H2O          6.648e+03    2.69        63314.00
!     CH3+C3H7O-N2=iBuOH       1.000e+13    0.00        0.00
!     C4H9Oi1+H=iBuOH          1.000e+14    0.00        0.00
!     C3H7-2+CH2OH=iBuOH       1.000e+13    0.00        0.00
!     C4H9Oi2+H=iBuOH          1.000e+14    0.00        0.00
!     iC4H9+OH=iBuOH           1.000e+13    0.00        0.00
!     C4H9Oi3+H=iBuOH          1.000e+14    0.00        0.00
!     C4H9Oi4+H=iBuOH          1.000e+14    0.00        0.00

iBuOH(+m)=iC4H8+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: ReactionLibrary: MRH-dehydration
      deltaHrxn(T=298K) = 7.658915338156689 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4947000e+01 1.9675000e-01 -2.1335000e-02 /
CHEB / 2.2224000e+01 3.7172000e-01 -3.8930000e-02 /
CHEB / -1.2150000e-01 3.1223000e-01 -2.8957000e-02 /
CHEB / -2.3917000e-01 2.3047000e-01 -1.5968000e-02 /
CHEB / -2.0784000e-01 1.4602000e-01 -3.8447000e-03 /

CH3+C3H7O-N2(+m)=iBuOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -90.35038445315479 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2566000e+01 3.7425000e-01 -3.6229000e-02 /
CHEB / -1.0158000e+00 6.7407000e-01 -5.7622000e-02 /
CHEB / -7.6657000e-01 4.8613000e-01 -2.3520000e-02 /
CHEB / -4.7782000e-01 2.6594000e-01 8.0793000e-03 /
CHEB / -2.6356000e-01 8.9218000e-02 2.1955000e-02 /

CH3+C3H7O-N2(+m)=iC4H8+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -82.6914691149981 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1225000e+00 -1.4939000e+00 -3.5656000e-02 /
CHEB / 2.9208000e+00 8.7644000e-01 -4.7501000e-02 /
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CHEB / 4.7272000e-01 5.5092000e-01 2.0742000e-03 /
CHEB / -1.8012000e-01 2.1027000e-01 3.6297000e-02 /
CHEB / -2.2095000e-01 -1.0688000e-02 3.5794000e-02 /

C4H9Oi1+H(+m)=iBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -102.14883252827838 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3465000e+01 4.7865000e-01 -5.0267000e-02 /
CHEB / -1.2828000e+00 8.1796000e-01 -6.4777000e-02 /
CHEB / -8.7374000e-01 5.0769000e-01 -1.2940000e-03 /
CHEB / -4.8089000e-01 2.0333000e-01 3.6892000e-02 /
CHEB / -2.1037000e-01 1.4246000e-02 3.5584000e-02 /

C4H9Oi1+H(+m)=iC4H8+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -94.48991719012167 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6439000e+00 -1.4098000e+00 -4.8825000e-02 /
CHEB / 2.3275000e+00 9.6635000e-01 -4.8867000e-02 /
CHEB / 3.1512000e-01 5.1266000e-01 2.8100000e-02 /
CHEB / -1.4390000e-01 1.1763000e-01 5.6313000e-02 /
CHEB / -1.4079000e-01 -7.2626000e-02 3.2472000e-02 /

C4H9Oi1+H(+m)=CH3+C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -11.798448075123586 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1742000e+01 -1.3124000e+00 -5.7050000e-02 /
CHEB / 2.1741000e+00 1.0563000e+00 -3.9556000e-02 /
CHEB / 3.3244000e-01 4.4338000e-01 5.6686000e-02 /
CHEB / -1.6353000e-01 4.7754000e-03 6.4080000e-02 /
CHEB / -1.1909000e-01 -1.2680000e-01 1.4594000e-02 /

C3H7-2+CH2OH(+m)=iBuOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -90.50077429979366 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2623000e+01 3.7425000e-01 -3.6229000e-02 /
CHEB / -1.0850000e+00 6.7407000e-01 -5.7622000e-02 /
CHEB / -7.7154000e-01 4.8613000e-01 -2.3520000e-02 /
CHEB / -4.9674000e-01 2.6594000e-01 8.0793000e-03 /
CHEB / -2.7306000e-01 8.9218000e-02 2.1955000e-02 /

C3H7-2+CH2OH(+m)=iC4H8+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -82.84185896163697 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1803000e+00 -1.4939000e+00 -3.5656000e-02 /
CHEB / 2.8516000e+00 8.7644000e-01 -4.7501000e-02 /
CHEB / 4.6775000e-01 5.5092000e-01 2.0742000e-03 /
CHEB / -1.9904000e-01 2.1027000e-01 3.6297000e-02 /
CHEB / -2.3044000e-01 -1.0688000e-02 3.5794000e-02 /
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C3H7-2+CH2OH(+m)=CH3+C3H7O-N2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -0.15038984663888222
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4152000e+00 -1.3845000e+00 -4.3755000e-02 /
CHEB / 3.5541000e+00 1.0053000e+00 -4.4353000e-02 /
CHEB / 3.8300000e-01 5.1047000e-01 3.0904000e-02 /
CHEB / -2.7082000e-01 8.2741000e-02 5.7949000e-02 /
CHEB / -1.9288000e-01 -1.0500000e-01 2.9386000e-02 /

C4H9Oi1+H(+m)=C3H7-2+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -11.648058228484702 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1681000e+01 -1.3124000e+00 -5.7050000e-02 /
CHEB / 2.0098000e+00 1.0563000e+00 -3.9556000e-02 /
CHEB / 2.8925000e-01 4.4338000e-01 5.6686000e-02 /
CHEB / -1.7866000e-01 4.7754000e-03 6.4080000e-02 /
CHEB / -1.2505000e-01 -1.2680000e-01 1.4594000e-02 /

C4H9Oi2+H(+m)=iBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -97.4893982241698 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3414000e+01 4.3373000e-01 -4.3285000e-02 /
CHEB / -1.1112000e+00 7.6130000e-01 -6.2610000e-02 /
CHEB / -8.4197000e-01 5.0715000e-01 -1.2972000e-02 /
CHEB / -4.9683000e-01 2.3547000e-01 2.4369000e-02 /
CHEB / -2.4241000e-01 4.5566000e-02 3.1632000e-02 /

C4H9Oi2+H(+m)=iC4H8+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -89.83048288601313 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3656000e+00 -1.4468000e+00 -4.1999000e-02 /
CHEB / 2.6101000e+00 9.3189000e-01 -4.9166000e-02 /
CHEB / 3.6349000e-01 5.3507000e-01 1.5384000e-02 /
CHEB / -1.7262000e-01 1.5780000e-01 4.8613000e-02 /
CHEB / -1.7971000e-01 -5.0667000e-02 3.5823000e-02 /

C4H9Oi2+H(+m)=CH3+C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -7.1390137710150245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1173000e+01 -1.3449000e+00 -5.0077000e-02 /
CHEB / 2.7242000e+00 1.0380000e+00 -4.2772000e-02 /
CHEB / 3.6295000e-01 4.7566000e-01 4.4850000e-02 /
CHEB / -2.1116000e-01 3.6093000e-02 6.2830000e-02 /
CHEB / -1.5174000e-01 -1.2124000e-01 2.1779000e-02 /

C4H9Oi2+H(+m)=C4H9Oi1+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = 4.659434304108565 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4241000e+00 -1.2759000e+00 -6.3183000e-02 /
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CHEB / 5.3007000e+00 1.0769000e+00 -3.5022000e-02 /
CHEB / 6.7268000e-01 4.0549000e-01 6.8479000e-02 /
CHEB / -6.0537000e-02 -3.0537000e-02 6.3203000e-02 /
CHEB / -7.1990000e-02 -1.3180000e-01 5.7751000e-03 /

C4H9Oi2+H(+m)=C3H7-2+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -6.9886239243761406 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1112000e+01 -1.3449000e+00 -5.0077000e-02 /
CHEB / 2.5599000e+00 1.0380000e+00 -4.2772000e-02 /
CHEB / 3.1976000e-01 4.7566000e-01 4.4850000e-02 /
CHEB / -2.2629000e-01 3.6093000e-02 6.2830000e-02 /
CHEB / -1.5769000e-01 -1.2124000e-01 2.1779000e-02 /

iC4H9+OH(+m)=iBuOH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -96.16987720184662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2536000e+01 4.2208000e-01 -4.1744000e-02 /
CHEB / -1.1674000e+00 7.4511000e-01 -6.1752000e-02 /
CHEB / -8.2716000e-01 5.0484000e-01 -1.5482000e-02 /
CHEB / -4.9301000e-01 2.4281000e-01 2.1041000e-02 /
CHEB / -2.4502000e-01 5.4227000e-02 3.0055000e-02 /

iC4H9+OH(+m)=iC4H8+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -88.51096186368993 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4197000e+00 -1.4561000e+00 -4.0554000e-02 /
CHEB / 2.5890000e+00 9.2177000e-01 -4.8951000e-02 /
CHEB / 3.8368000e-01 5.3949000e-01 1.2434000e-02 /
CHEB / -1.7309000e-01 1.6840000e-01 4.6307000e-02 /
CHEB / -1.8514000e-01 -4.3709000e-02 3.6234000e-02 /

iC4H9+OH(+m)=CH3+C3H7O-N2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.819492748691827 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0135000e+01 -1.3529000e+00 -4.8607000e-02 /
CHEB / 2.7929000e+00 1.0322000e+00 -4.3243000e-02 /
CHEB / 3.7399000e-01 4.8330000e-01 4.1916000e-02 /
CHEB / -2.1778000e-01 4.4940000e-02 6.2116000e-02 /
CHEB / -1.5533000e-01 -1.1887000e-01 2.3480000e-02 /

C4H9Oi1+H(+m)=iC4H9+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.978955326431759 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7582000e+00 -1.2833000e+00 -6.1780000e-02 /
CHEB / 3.0841000e+00 1.0734000e+00 -3.6099000e-02 /
CHEB / 5.0639000e-01 4.1344000e-01 6.6082000e-02 /
CHEB / -1.0929000e-01 -2.4036000e-02 6.3601000e-02 /
CHEB / -8.7789000e-02 -1.3140000e-01 7.5807000e-03 /
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iC4H9+OH(+m)=C3H7-2+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.669102902052943 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0074000e+01 -1.3529000e+00 -4.8607000e-02 /
CHEB / 2.6286000e+00 1.0322000e+00 -4.3243000e-02 /
CHEB / 3.3080000e-01 4.8330000e-01 4.1916000e-02 /
CHEB / -2.3291000e-01 4.4940000e-02 6.2116000e-02 /
CHEB / -1.6128000e-01 -1.1887000e-01 2.3480000e-02 /

C4H9Oi2+H(+m)=iC4H9+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -1.3195210223231975 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0837000e+00 -1.3148000e+00 -5.4890000e-02 /
CHEB / 3.7598000e+00 1.0592000e+00 -4.0421000e-02 /
CHEB / 5.0427000e-01 4.4623000e-01 5.5197000e-02 /
CHEB / -1.5579000e-01 3.1412000e-03 6.4310000e-02 /
CHEB / -1.1672000e-01 -1.2928000e-01 1.4933000e-02 /

C4H9Oi3+H(+m)=iBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -96.18958336897245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3476000e+01 4.1641000e-01 -4.1027000e-02 /
CHEB / -1.0915000e+00 7.3706000e-01 -6.1306000e-02 /
CHEB / -8.1466000e-01 5.0340000e-01 -1.6622000e-02 /
CHEB / -4.8891000e-01 2.4616000e-01 1.9433000e-02 /
CHEB / -2.4276000e-01 5.8463000e-02 2.9218000e-02 /

C4H9Oi3+H(+m)=iC4H8+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -88.53066803081576 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3253000e+00 -1.4606000e+00 -3.9892000e-02 /
CHEB / 2.6831000e+00 9.1669000e-01 -4.8819000e-02 /
CHEB / 3.9900000e-01 5.4141000e-01 1.1060000e-02 /
CHEB / -1.7124000e-01 1.7353000e-01 4.5156000e-02 /
CHEB / -1.8443000e-01 -4.0152000e-02 3.6360000e-02 /

C4H9Oi3+H(+m)=CH3+C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.83919891581766 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0992000e+01 -1.3568000e+00 -4.7937000e-02 /
CHEB / 2.9346000e+00 1.0292000e+00 -4.3434000e-02 /
CHEB / 3.8387000e-01 4.8688000e-01 4.0522000e-02 /
CHEB / -2.1906000e-01 4.9318000e-02 6.1719000e-02 /
CHEB / -1.5370000e-01 -1.1757000e-01 2.4273000e-02 /

C4H9Oi1+H(+m)=C4H9Oi3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.9592491593059265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3135000e+00 -1.2869000e+00 -6.1136000e-02 /
CHEB / 3.5701000e+00 1.0716000e+00 -3.6582000e-02 /
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CHEB / 6.4456000e-01 4.1722000e-01 6.4928000e-02 /
CHEB / -6.0614000e-02 -2.0785000e-02 6.3752000e-02 /
CHEB / -6.9785000e-02 -1.3111000e-01 8.4492000e-03 /

C4H9Oi3+H(+m)=C3H7-2+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -5.688809069178776 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0932000e+01 -1.3568000e+00 -4.7937000e-02 /
CHEB / 2.7702000e+00 1.0292000e+00 -4.3434000e-02 /
CHEB / 3.4068000e-01 4.8688000e-01 4.0522000e-02 /
CHEB / -2.3419000e-01 4.9318000e-02 6.1719000e-02 /
CHEB / -1.5965000e-01 -1.1757000e-01 2.4273000e-02 /

C4H9Oi2+H(+m)=C4H9Oi3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -1.2998148551973614 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6519000e+00 -1.3185000e+00 -5.4229000e-02 /
CHEB / 4.2299000e+00 1.0569000e+00 -4.0771000e-02 /
CHEB / 6.4716000e-01 4.5001000e-01 5.3909000e-02 /
CHEB / -1.0765000e-01 6.8962000e-03 6.4236000e-02 /
CHEB / -9.9086000e-02 -1.2862000e-01 1.5805000e-02 /

C4H9Oi3+H(+m)=iC4H9+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -0.019706167125832508
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8516000e+00 -1.3263000e+00 -5.2769000e-02 /
CHEB / 4.0343000e+00 1.0521000e+00 -4.1476000e-02 /
CHEB / 5.0550000e-01 4.5793000e-01 5.1131000e-02 /
CHEB / -1.6141000e-01 1.4836000e-02 6.3994000e-02 /
CHEB / -1.1748000e-01 -1.2718000e-01 1.7619000e-02 /

C4H9Oi4+H(+m)=iBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (iBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -104.64886704332415 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3371000e+01 5.0831000e-01 -5.6017000e-02 /
CHEB / -1.3170000e+00 8.4904000e-01 -6.4637000e-02 /
CHEB / -8.9989000e-01 5.0151000e-01 7.7895000e-03 /
CHEB / -4.9521000e-01 1.8080000e-01 4.4167000e-02 /
CHEB / -2.0742000e-01 -3.2995000e-03 3.6244000e-02 /

C4H9Oi4+H(+m)=iC4H8+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -96.98995170516747 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6724000e+00 -1.3847000e+00 -5.4614000e-02 /
CHEB / 2.2376000e+00 9.8403000e-01 -4.7122000e-02 /
CHEB / 2.8073000e-01 4.9425000e-01 3.7176000e-02 /
CHEB / -1.5275000e-01 9.3250000e-02 5.9919000e-02 /
CHEB / -1.3591000e-01 -8.2815000e-02 2.9061000e-02 /
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C4H9Oi4+H(+m)=CH3+C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -14.29848259016937 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1917000e+01 -1.2897000e+00 -6.2894000e-02 /
CHEB / 1.9583000e+00 1.0641000e+00 -3.5741000e-02 /
CHEB / 3.0102000e-01 4.2076000e-01 6.4456000e-02 /
CHEB / -1.6410000e-01 -1.2651000e-02 6.3506000e-02 /
CHEB / -1.1757000e-01 -1.2776000e-01 9.6613000e-03 /

C4H9Oi4+H(+m)=C4H9Oi1+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -2.5000345150457832 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5147000e+00 -1.2246000e+00 -7.5146000e-02 /
CHEB / 4.1155000e+00 1.0891000e+00 -2.4281000e-02 /
CHEB / 7.2764000e-01 3.5192000e-01 8.3514000e-02 /
CHEB / -2.5428000e-02 -6.4577000e-02 5.7807000e-02 /
CHEB / -4.7432000e-02 -1.2890000e-01 -5.6178000e-03 /

C4H9Oi4+H(+m)=C3H7-2+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -14.148092743530485 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1856000e+01 -1.2897000e+00 -6.2894000e-02 /
CHEB / 1.7940000e+00 1.0641000e+00 -3.5741000e-02 /
CHEB / 2.5783000e-01 4.2076000e-01 6.4456000e-02 /
CHEB / -1.7923000e-01 -1.2651000e-02 6.3506000e-02 /
CHEB / -1.2352000e-01 -1.2776000e-01 9.6613000e-03 /

C4H9Oi4+H(+m)=C4H9Oi2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -7.159468819154348 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1671000e+00 -1.2540000e+00 -6.8884000e-02 /
CHEB / 3.2728000e+00 1.0815000e+00 -3.0322000e-02 /
CHEB / 5.9182000e-01 3.8320000e-01 7.5211000e-02 /
CHEB / -7.3403000e-02 -4.4670000e-02 6.1276000e-02 /
CHEB / -7.2518000e-02 -1.3070000e-01 1.0233000e-03 /

C4H9Oi4+H(+m)=iC4H9+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -8.478989841477542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9846000e+00 -1.2613000e+00 -6.7525000e-02 /
CHEB / 2.8110000e+00 1.0786000e+00 -3.1566000e-02 /
CHEB / 4.8623000e-01 3.9100000e-01 7.3046000e-02 /
CHEB / -1.0889000e-01 -3.8811000e-02 6.1916000e-02 /
CHEB / -8.8353000e-02 -1.3064000e-01 2.7634000e-03 /

C4H9Oi4+H(+m)=C4H9Oi3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (iBuOH)  deltaHrxn(T=298K) = -8.45928367435171 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5334000e+00 -1.2648000e+00 -6.6899000e-02 /
CHEB / 3.3045000e+00 1.0771000e+00 -3.2133000e-02 /
CHEB / 6.2265000e-01 3.9473000e-01 7.2000000e-02 /
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CHEB / -6.0197000e-02 -3.5876000e-02 6.2190000e-02 /
CHEB / -7.0102000e-02 -1.3052000e-01 3.6049000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tBuOH       -75.87      78.3  28.26 35.02 40.83 45.65 53.18 58.85
      67.96  !MRH CBS-QB3 w/1DHR corrections
!     iC4H8       -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34 54.27
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tC4H9       14.3  76.21 21.71 26.64 31.62 36.12 43.55 49.22 58.13
!     OC[CH3]3    -21.12      76.85 27.25 33.57 38.95 43.42 50.47 55.8
      64.28  !MRH CBS-QB3 w/1DHR corrections
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3C[OH]CH3 -22.33      74.56 21.77 26.05 29.95 33.3  38.64 42.68
      49.13
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     tBuOH=iC4H8+H2O         7.564e+05    2.42        61825.00
!     OH+tC4H9=tBuOH          8.000e+12    0.00        0.00
!     OC[CH3]3+H=tBuOH        1.000e+14    0.00        0.00
!     CH3C[OH]CH3+CH3=tBuOH   8.000e+12    0.00        0.00
!     HOC[CH2][CH3]2+H=tBuOH  1.000e+14    0.00        0.00

tBuOH(+m)=iC4H8+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (tBuOH) High-P Limit: ReactionLibrary: MRH-dehydration
      deltaHrxn(T=298K) = 15.188289658800187 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3071000e+01 2.8456000e-01 -3.6796000e-02 /
CHEB / 2.1440000e+01 5.3247000e-01 -6.5209000e-02 /
CHEB / -2.5279000e-01 4.3331000e-01 -4.3171000e-02 /
CHEB / -3.1307000e-01 2.9977000e-01 -1.5355000e-02 /
CHEB / -2.3982000e-01 1.6673000e-01 9.0900000e-03 /

OH+tC4H9(+m)=tBuOH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (tBuOH) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -98.84990085846324 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2368000e+01 5.0497000e-01 -5.4489000e-02 /
CHEB / -1.3187000e+00 8.6890000e-01 -7.1740000e-02 /
CHEB / -8.9086000e-01 5.4164000e-01 1.2502000e-03 /
CHEB / -5.1457000e-01 2.0775000e-01 5.0406000e-02 /
CHEB / -2.2855000e-01 -7.3622000e-03 5.1604000e-02 /
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OH+tC4H9(+m)=iC4H8+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -83.66161119966306 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0073000e+01 -1.4180000e+00 -5.0595000e-02 /
CHEB / 2.1994000e+00 9.6833000e-01 -5.5456000e-02 /
CHEB / 2.9045000e-01 5.3326000e-01 2.6037000e-02 /
CHEB / -1.8388000e-01 1.3151000e-01 6.4824000e-02 /
CHEB / -1.7370000e-01 -7.8241000e-02 4.3879000e-02 /

OC[CH3]3+H(+m)=tBuOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -106.83863940345452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3473000e+01 5.6539000e-01 -6.6090000e-02 /
CHEB / -1.4819000e+00 9.2298000e-01 -6.6920000e-02 /
CHEB / -9.0908000e-01 5.1270000e-01 2.5096000e-02 /
CHEB / -4.7582000e-01 1.4966000e-01 6.5545000e-02 /
CHEB / -1.8021000e-01 -4.3443000e-02 4.7059000e-02 /

OC[CH3]3+H(+m)=iC4H8+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -91.65034974465433 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1492000e+01 -1.3621000e+00 -6.3591000e-02 /
CHEB / 1.8807000e+00 1.0044000e+00 -4.9995000e-02 /
CHEB / 2.3573000e-01 4.8716000e-01 4.7998000e-02 /
CHEB / -1.4134000e-01 7.4303000e-02 7.2152000e-02 /
CHEB / -1.2288000e-01 -9.8621000e-02 3.3081000e-02 /

OC[CH3]3+H(+m)=OH+tC4H9(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -7.9887385449912784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8380000e+00 -1.2428000e+00 -7.6715000e-02 /
CHEB / 2.3394000e+00 1.0824000e+00 -3.0157000e-02 /
CHEB / 4.2836000e-01 3.7516000e-01 8.3269000e-02 /
CHEB / -1.1675000e-01 -4.9947000e-02 6.6557000e-02 /
CHEB / -9.6537000e-02 -1.3233000e-01 6.7045000e-04 /

CH3C[OH]CH3+CH3(+m)=tBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -88.7805786529322 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2366000e+01 4.3732000e-01 -4.7772000e-02 /
CHEB / -1.0202000e+00 7.8066000e-01 -7.2953000e-02 /
CHEB / -7.9765000e-01 5.4446000e-01 -2.1260000e-02 /
CHEB / -4.8461000e-01 2.7027000e-01 2.6113000e-02 /
CHEB / -2.4648000e-01 5.4857000e-02 4.5524000e-02 /

CH3C[OH]CH3+CH3(+m)=iC4H8+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -73.59228899413202 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4998000e+00 -1.4757000e+00 -4.2648000e-02 /
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CHEB / 2.8163000e+00 9.0705000e-01 -5.6170000e-02 /
CHEB / 4.5451000e-01 5.6564000e-01 5.2241000e-03 /
CHEB / -1.6958000e-01 2.0476000e-01 4.8859000e-02 /
CHEB / -2.0618000e-01 -3.1929000e-02 4.8445000e-02 /

OH+tC4H9(+m)=CH3C[OH]CH3+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -10.069322205531037 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0589000e+01 -1.3417000e+00 -5.5624000e-02 /
CHEB / 2.2350000e+00 1.0424000e+00 -4.7399000e-02 /
CHEB / 3.4984000e-01 4.7822000e-01 5.0060000e-02 /
CHEB / -2.0430000e-01 3.4001000e-02 7.2541000e-02 /
CHEB / -1.6170000e-01 -1.2750000e-01 2.7340000e-02 /

OC[CH3]3+H(+m)=CH3C[OH]CH3+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -18.058060750522316 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2389000e+01 -1.2892000e+00 -6.9038000e-02 /
CHEB / 1.5862000e+00 1.0619000e+00 -3.8539000e-02 /
CHEB / 2.8899000e-01 4.2499000e-01 6.9328000e-02 /
CHEB / -1.4097000e-01 -9.2919000e-03 7.1332000e-02 /
CHEB / -1.1451000e-01 -1.3019000e-01 1.3672000e-02 /

HOC[CH2][CH3]2+H(+m)=tBuOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -103.21871438096564 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3510000e+01 5.2974000e-01 -5.8474000e-02 /
CHEB / -1.3781000e+00 8.9462000e-01 -7.0552000e-02 /
CHEB / -8.8176000e-01 5.3196000e-01 1.0915000e-02 /
CHEB / -4.6241000e-01 1.8271000e-01 5.7757000e-02 /
CHEB / -1.8177000e-01 -2.4871000e-02 5.0684000e-02 /

HOC[CH2][CH3]2+H(+m)=iC4H8+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -88.03042472216545 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1362000e+01 -1.3954000e+00 -5.5187000e-02 /
CHEB / 2.0651000e+00 9.8611000e-01 -5.4166000e-02 /
CHEB / 2.8218000e-01 5.1542000e-01 3.5034000e-02 /
CHEB / -1.2929000e-01 1.0591000e-01 6.8892000e-02 /
CHEB / -1.2515000e-01 -8.9004000e-02 3.9904000e-02 /

HOC[CH2][CH3]2+H(+m)=OH+tC4H9(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -4.368813522502389 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3673000e+00 -1.2728000e+00 -6.8463000e-02 /
CHEB / 2.8516000e+00 1.0789000e+00 -3.7843000e-02 /
CHEB / 4.5154000e-01 4.0549000e-01 7.4232000e-02 /
CHEB / -1.1758000e-01 -3.2640000e-02 7.0373000e-02 /
CHEB / -9.2671000e-02 -1.3532000e-01 7.9156000e-03 /
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OC[CH3]3+H(+m)=HOC[CH2][CH3]2+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tBuOH)  deltaHrxn(T=298K) = -3.619925022488893 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0508000e+00 -1.2241000e+00 -8.0802000e-02 /
CHEB / 3.9040000e+00 1.0861000e+00 -2.5783000e-02 /
CHEB / 7.8347000e-01 3.5516000e-01 8.8517000e-02 /
CHEB / 4.2356000e-03 -6.1789000e-02 6.3689000e-02 /
CHEB / -4.5423000e-02 -1.3049000e-01 -4.0275000e-03 /

HOC[CH2][CH3]2+H(+m)=CH3C[OH]CH3+CH3(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tBuOH)   deltaHrxn(T=298K) = -14.438135728033423
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2063000e+01 -1.3207000e+00 -6.0432000e-02 /
CHEB / 1.9359000e+00 1.0531000e+00 -4.4770000e-02 /
CHEB / 3.4169000e-01 4.5655000e-01 5.8177000e-02 /
CHEB / -1.3866000e-01 1.3985000e-02 7.2848000e-02 /
CHEB / -1.1494000e-01 -1.3005000e-01 2.1671000e-02 /



!PDepNetwork C4H8-1
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H7-11           58.99 75.0  20.38 25.34 29.68 33.36 39.14 43.48
      50.22 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H7-12           56.79 75.42 20.23 24.88 29.1  32.76 38.62 43.06
      49.99 null
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!Here are the path reactions and their high-P limit kinetics:
!     C4H7-11+H=C4H8-1        5.3600000e+14      0.00000
9.8000000e+02
!     C2H3+C2H5=C4H8-1        1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7-12+H=C4H8-1        1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+CH3=C4H8-1        2.4874006e+15      -0.90000
2.5000000e+02
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!     C4H7-24+H=C4H8-1        5.0000000e+13      0.00000
0.0000000e+00
!     C4H7-14+H=C4H8-1        1.0000000e+14      0.00000
0.0000000e+00

C4H7-11+H(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination exact:  Cd_pri_rad
H_rad       deltaHrxn(T=298K) = -109.19833171991216 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1228000e+01 3.5206000e+00 -1.0799000e+00 /
CHEB / -1.5994000e+00 7.4811000e-01 3.2090000e-01 /
CHEB / -1.4135000e+00 5.0296000e-01 1.5472000e-01 /
CHEB / -7.9657000e-01 1.6226000e-01 6.7930000e-02 /
CHEB / -4.2927000e-01 1.7986000e-02 2.4726000e-02 /

C4H7-11+H(+m)=C2H3+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -9.458648414262289 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1524000e+01 -5.4112000e-01 -2.1538000e-01 /
CHEB / 2.0866000e+00 5.3993000e-01 1.8986000e-01 /
CHEB / 5.4269000e-01 9.4532000e-02 6.0279000e-02 /
CHEB / 6.3472000e-02 -5.4957000e-02 -9.0476000e-03 /
CHEB / -2.9031000e-02 -3.9019000e-02 -1.9982000e-02 /

C4H7-11+H(+m)=C4H7-12+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -2.1997755775516694 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4782000e+00 -5.1853000e-01 -2.0662000e-01 /
CHEB / 3.5155000e+00 5.3854000e-01 1.8840000e-01 /
CHEB / 8.5613000e-01 6.5330000e-02 5.3327000e-02 /
CHEB / 1.3937000e-01 -5.5226000e-02 -1.2668000e-02 /
CHEB / 3.8420000e-03 -3.2830000e-02 -1.9154000e-02 /

C4H7-11+H(+m)=aC3H5+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -33.79641660147227 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3961000e+01 -5.2330000e-01 -2.3889000e-01 /
CHEB / 5.3735000e-01 4.6401000e-01 1.9382000e-01 /
CHEB / 8.2618000e-03 1.4534000e-01 7.6032000e-02 /
CHEB / -6.2002000e-02 -2.6635000e-02 2.0343000e-03 /
CHEB / -6.0048000e-02 -4.4904000e-02 -1.8757000e-02 /

C4H7-11+H(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -24.207486076651143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1569000e+01 -5.3831000e-01 -2.3243000e-01 /
CHEB / 1.8168000e+00 4.9127000e-01 1.9229000e-01 /
CHEB / 4.0460000e-01 1.3788000e-01 7.2077000e-02 /
CHEB / 7.0148000e-02 -3.5444000e-02 -8.1588000e-04 /
CHEB / -1.3797000e-02 -4.5638000e-02 -1.9359000e-02 /
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C4H7-11+H(+m)=C4H7-14+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -10.098901301946107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0698000e+01 -5.4417000e-01 -2.1814000e-01 /
CHEB / 2.7076000e+00 5.3528000e-01 1.9031000e-01 /
CHEB / 7.0853000e-01 1.0341000e-01 6.2291000e-02 /
CHEB / 1.3302000e-01 -5.3122000e-02 -7.7880000e-03 /
CHEB / -9.3509000e-04 -4.0895000e-02 -2.0058000e-02 /

C2H3+C2H5(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     C_rad/H2/Cs           deltaHrxn(T=298K) = -
99.73968330564988 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0846000e+01 1.8944000e+00 -6.1518000e-01 /
CHEB / -1.8561000e+00 1.0421000e+00 1.4092000e-01 /
CHEB / -1.3387000e+00 6.0830000e-01 8.3323000e-02 /
CHEB / -7.6803000e-01 2.0997000e-01 6.4363000e-02 /
CHEB / -4.2912000e-01 3.6139000e-02 3.2928000e-02 /

C2H3+C2H5(+m)=aC3H5+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -24.337768187209974 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2022000e+01 -8.3862000e-01 -2.3272000e-01 /
CHEB / 4.5487000e-01 7.2540000e-01 1.5080000e-01 /
CHEB / 6.0612000e-02 2.3290000e-01 9.4293000e-02 /
CHEB / -7.4972000e-02 -2.4825000e-02 2.7407000e-02 /
CHEB / -8.1408000e-02 -6.3508000e-02 -1.3158000e-02 /

C2H3+C2H5(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -14.748837662388858 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4518000e+00 -8.3421000e-01 -2.2161000e-01 /
CHEB / 1.8651000e+00 7.5149000e-01 1.4666000e-01 /
CHEB / 4.8099000e-01 2.0973000e-01 9.2257000e-02 /
CHEB / 5.3258000e-02 -4.1448000e-02 2.2241000e-02 /
CHEB / -3.6960000e-02 -6.3898000e-02 -1.6667000e-02 /

C4H7-12+H(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
106.9985561423605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0213000e+01 2.8992000e+00 -9.3559000e-01 /
CHEB / -2.0437000e+00 8.5787000e-01 2.7844000e-01 /
CHEB / -1.4046000e+00 5.4686000e-01 1.3304000e-01 /
CHEB / -7.9488000e-01 1.8032000e-01 6.6853000e-02 /
CHEB / -4.3290000e-01 2.4021000e-02 2.7118000e-02 /

C4H7-12+H(+m)=C2H3+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -7.258872836710626 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 9.6743000e+00 -6.1903000e-01 -2.1792000e-01 /
CHEB / 1.9149000e+00 6.1990000e-01 1.8350000e-01 /
CHEB / 5.5842000e-01 1.0198000e-01 6.8734000e-02 /
CHEB / 4.1776000e-02 -5.9287000e-02 -5.1939000e-03 /
CHEB / -3.9821000e-02 -4.2692000e-02 -2.1361000e-02 /

C4H7-12+H(+m)=aC3H5+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -31.596641023920604 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2358000e+01 -6.2663000e-01 -2.4806000e-01 /
CHEB / 1.4873000e-01 5.5079000e-01 1.9114000e-01 /
CHEB / 1.1378000e-02 1.7405000e-01 8.4084000e-02 /
CHEB / -7.2497000e-02 -2.6990000e-02 9.2770000e-03 /
CHEB / -7.0198000e-02 -5.1543000e-02 -1.8056000e-02 /

C4H7-12+H(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -22.00771049909948 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9111000e+00 -6.3709000e-01 -2.3877000e-01 /
CHEB / 1.4666000e+00 5.7880000e-01 1.8782000e-01 /
CHEB / 4.1632000e-01 1.6215000e-01 7.9978000e-02 /
CHEB / 5.9114000e-02 -3.8265000e-02 5.6661000e-03 /
CHEB / -2.4536000e-02 -5.2215000e-02 -1.9323000e-02 /

C4H7-12+H(+m)=C4H7-14+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -7.899125724394445 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8849000e+00 -6.2774000e-01 -2.2062000e-01 /
CHEB / 2.4958000e+00 6.1973000e-01 1.8344000e-01 /
CHEB / 7.2828000e-01 1.1324000e-01 7.0808000e-02 /
CHEB / 1.1352000e-01 -5.8138000e-02 -3.3929000e-03 /
CHEB / -1.2325000e-02 -4.5002000e-02 -2.1329000e-02 /

aC3H5+CH3(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_methyl       deltaHrxn(T=298K) = -
75.4019151184399 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2412000e+01 3.7483000e-01 -3.3378000e-02 /
CHEB / -1.5142000e+00 6.7301000e-01 -4.8752000e-02 /
CHEB / -9.5012000e-01 4.8550000e-01 -1.0224000e-02 /
CHEB / -6.1566000e-01 2.7514000e-01 2.1268000e-02 /
CHEB / -3.9204000e-01 1.1262000e-01 3.1224000e-02 /

C4H7-24+H(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
84.99084564326101 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3150000e+01 5.5123000e-01 -7.6800000e-02 /
CHEB / -1.4876000e+00 9.1109000e-01 -8.2880000e-02 /
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CHEB / -1.0188000e+00 5.7552000e-01 -9.5088000e-04 /
CHEB / -6.6610000e-01 2.7239000e-01 4.0951000e-02 /
CHEB / -4.0473000e-01 8.6345000e-02 3.9413000e-02 /

C4H7-24+H(+m)=aC3H5+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -9.588930524821109 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2184000e+01 -1.3137000e+00 -7.8735000e-02 /
CHEB / 1.3818000e+00 1.0091000e+00 -4.2269000e-02 /
CHEB / 2.7617000e-01 4.2437000e-01 6.6491000e-02 /
CHEB / -1.3043000e-01 4.2612000e-02 6.9424000e-02 /
CHEB / -1.2152000e-01 -7.8179000e-02 2.0978000e-02 /

C4H7-14+H(+m)=C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -99.09943041796605
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2523000e+01 1.5914000e+00 -4.9808000e-01 /
CHEB / -1.8938000e+00 1.0899000e+00 8.0931000e-02 /
CHEB / -1.2850000e+00 6.2065000e-01 6.6298000e-02 /
CHEB / -7.5235000e-01 2.1917000e-01 6.3891000e-02 /
CHEB / -4.2213000e-01 4.1070000e-02 3.5292000e-02 /

C4H7-14+H(+m)=C2H3+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = 0.6402528876838254 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8430000e+00 -7.7097000e-01 -2.0842000e-01 /
CHEB / 3.1016000e+00 7.6254000e-01 1.4971000e-01 /
CHEB / 5.8234000e-01 1.2809000e-01 8.8836000e-02 /
CHEB / 1.5692000e-02 -6.0919000e-02 5.9454000e-03 /
CHEB / -4.6886000e-02 -5.2086000e-02 -2.2631000e-02 /

C4H7-14+H(+m)=aC3H5+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -23.697515299526145 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3385000e+01 -9.1974000e-01 -2.1596000e-01 /
CHEB / 4.6327000e-01 7.9018000e-01 1.2452000e-01 /
CHEB / 1.0489000e-01 2.5600000e-01 9.5925000e-02 /
CHEB / -7.2792000e-02 -2.2481000e-02 3.5221000e-02 /
CHEB / -8.0847000e-02 -6.7560000e-02 -1.0144000e-02 /

C4H7-14+H(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H8-1) deltaHrxn(T=298K) = -14.10858477470503 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0762000e+01 -9.0736000e-01 -2.0615000e-01 /
CHEB / 1.9166000e+00 8.1411000e-01 1.2157000e-01 /
CHEB / 5.3007000e-01 2.2771000e-01 9.5708000e-02 /
CHEB / 5.3225000e-02 -4.1319000e-02 2.9404000e-02 /
CHEB / -3.6741000e-02 -6.7822000e-02 -1.4846000e-02 /

!PDepNetwork C4H8-2
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!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+pC3H5=C4H8-2        7.2300000e+13      0.00000
0.0000000e+00
!     C4H7-24+H=C4H8-2        5.0000000e+13      0.00000
0.0000000e+00
!     C4H7-22+H=C4H8-2        1.4157154e+13      -0.15000
2.9166667e+02

CH3+pC3H5(+m)=C4H8-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2) High-P Limit: R_Recombination exact:  C_methyl
Cd_pri_rad        deltaHrxn(T=298K) = -101.58926025557103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3117000e+01 5.1179000e-01 -6.7300000e-02 /
CHEB / -1.4614000e+00 8.9933000e-01 -1.0045000e-01 /
CHEB / -1.1472000e+00 6.1262000e-01 -3.3614000e-02 /
CHEB / -7.5563000e-01 3.1594000e-01 1.5511000e-02 /
CHEB / -4.6441000e-01 1.1087000e-01 2.8152000e-02 /

CH3+pC3H5(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2)      deltaHrxn(T=298K) = -13.87861142683996
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1235000e+01 -1.3876000e+00 -4.7486000e-02 /
CHEB / 1.8383000e+00 9.9278000e-01 -4.5226000e-02 /
CHEB / 2.0934000e-01 5.0187000e-01 3.4598000e-02 /
CHEB / -1.7882000e-01 9.2996000e-02 5.9077000e-02 /
CHEB / -1.3957000e-01 -8.3467000e-02 2.9364000e-02 /

C4H7-24+H(+m)=C4H8-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
87.71064882873107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3257000e+01 2.8713000e-01 -2.5151000e-02 /
CHEB / -9.4469000e-01 5.3032000e-01 -4.1962000e-02 /
CHEB / -7.8421000e-01 4.1518000e-01 -2.1624000e-02 /
CHEB / -5.8615000e-01 2.6950000e-01 1.3115000e-04 /
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CHEB / -4.0376000e-01 1.3675000e-01 1.4093000e-02 /

C4H7-22+H(+m)=C4H8-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
106.60861926934487 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1708000e+01 6.3346000e-01 -9.7861000e-02 /
CHEB / -1.6690000e+00 1.0716000e+00 -1.3164000e-01 /
CHEB / -1.3008000e+00 6.7546000e-01 -3.1605000e-02 /
CHEB / -8.3098000e-01 3.1337000e-01 2.5528000e-02 /
CHEB / -4.8876000e-01 9.5108000e-02 3.0709000e-02 /

C4H7-22+H(+m)=CH3+pC3H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2)      deltaHrxn(T=298K) = -5.019359013773851
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0623000e+01 -1.2622000e+00 -6.8073000e-02 /
CHEB / 2.0817000e+00 1.0740000e+00 -3.2172000e-02 /
CHEB / 2.2889000e-01 3.8464000e-01 7.4463000e-02 /
CHEB / -1.5192000e-01 -3.1773000e-02 6.1131000e-02 /
CHEB / -8.8956000e-02 -1.1679000e-01 2.5149000e-03 /

C4H7-22+H(+m)=C4H7-24+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H8-2)      deltaHrxn(T=298K) = -18.897970440613797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0314000e+01 -1.3369000e+00 -5.9086000e-02 /
CHEB / 1.4890000e+00 1.0254000e+00 -4.1865000e-02 /
CHEB / 1.0908000e-01 4.5759000e-01 5.3199000e-02 /
CHEB / -1.7264000e-01 4.4157000e-02 6.3912000e-02 /
CHEB / -1.1894000e-01 -9.8354000e-02 2.0308000e-02 /

!PDepNetwork iC4H8
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     HCC[CH3]2         55.3  72.75 21.39 25.9  29.94 33.42 39.09 43.4
      50.18 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H7             35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62
      50.57
!Here are the path reactions and their high-P limit kinetics:
!     HCC[CH3]2+H=iC4H8             5.3600000e+14      0.00000
9.8000000e+02
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!     sC3H5+CH3=iC4H8          1.000e+13    0.00        0.00
!     iC4H7+H=iC4H8            5.0000000e+13      0.00000
0.0000000e+00

HCC[CH3]2+H(+m)=iC4H8(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (iC4H8) High-P Limit: R_Recombination exact:  Cd_pri_rad
H_rad       deltaHrxn(T=298K) = -109.60817449677965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3437000e+01 7.0718000e-01 -1.2353000e-01 /
CHEB / -1.3627000e+00 1.1255000e+00 -1.3306000e-01 /
CHEB / -1.2222000e+00 6.6576000e-01 -1.5258000e-02 /
CHEB / -7.5866000e-01 2.9039000e-01 3.6659000e-02 /
CHEB / -4.4300000e-01 8.7222000e-02 3.1482000e-02 /

HCC[CH3]2+H(+m)=sC3H5+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (iC4H8) deltaHrxn(T=298K) = -10.188704800842899 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2861000e+01 -1.2403000e+00 -8.5422000e-02 /
CHEB / 1.7819000e+00 1.0508000e+00 -2.4819000e-02 /
CHEB / 2.3586000e-01 3.6399000e-01 8.4462000e-02 /
CHEB / -9.8531000e-02 -2.0842000e-02 6.1551000e-02 /
CHEB / -6.7795000e-02 -9.9998000e-02 1.8416000e-03 /

HCC[CH3]2+H(+m)=iC4H7+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (iC4H8) deltaHrxn(T=298K) = -20.09765691088011 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2008000e+01 -1.2897000e+00 -7.9895000e-02 /
CHEB / 1.7364000e+00 1.0235000e+00 -3.3430000e-02 /
CHEB / 2.0411000e-01 4.1182000e-01 7.1424000e-02 /
CHEB / -8.9782000e-02 2.2892000e-02 6.6228000e-02 /
CHEB / -7.4276000e-02 -8.9843000e-02 1.3746000e-02 /

sC3H5+CH3(+m)=iC4H8(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#35 (iC4H8) High-P Limit: R_Recombination Primary Kinetic Library: Mike
      deltaHrxn(T=298K) = -99.41946969593675 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2518000e+01 4.2463000e-01 -4.7597000e-02 /
CHEB / -1.2968000e+00 7.5871000e-01 -7.2821000e-02 /
CHEB / -9.6257000e-01 5.3999000e-01 -2.5409000e-02 /
CHEB / -6.5129000e-01 3.0025000e-01 1.2905000e-02 /
CHEB / -4.1643000e-01 1.2138000e-01 2.5323000e-02 /

sC3H5+CH3(+m)=iC4H7+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (iC4H8) deltaHrxn(T=298K) = -9.908952110037212 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9647000e+00 -1.4172000e+00 -4.5487000e-02 /
CHEB / 2.1799000e+00 9.6176000e-01 -4.7810000e-02 /
CHEB / 3.6016000e-01 5.1699000e-01 2.6911000e-02 /
CHEB / -1.4727000e-01 1.2742000e-01 5.6275000e-02 /
CHEB / -1.3229000e-01 -6.0239000e-02 3.3928000e-02 /
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iC4H7+H(+m)=iC4H8(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#35 (iC4H8) High-P Limit: R_Recombination estimate: (Average:)
C_rad/H2/Cd     H_rad         deltaHrxn(T=298K) = -89.51051758589955
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3415000e+01 2.7612000e-01 -2.1890000e-02 /
CHEB / -9.6308000e-01 5.1056000e-01 -3.6119000e-02 /
CHEB / -7.1790000e-01 4.0137000e-01 -1.7512000e-02 /
CHEB / -5.3627000e-01 2.6324000e-01 2.1846000e-03 /
CHEB / -3.7030000e-01 1.3723000e-01 1.4489000e-02 /

!PDepNetwork nC4H8O && C4H8O-enol
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  Estimated by Group Additivity
!     C4H8O-enol        -42.24      81.3  24.52 30.69 35.99 40.36 47.01
      51.87 59.46 Estimated by Group Additivity
!     CH3               35.1  46.36 9.2   9.98  10.75 11.5  12.86 14.08
      16.29 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009089)
!     C3H5O-enol2             -1.38 69.74 18.78 23.27 26.89 29.75 33.95
      36.93 41.61 Estimated by Group Additivity
!     C4H7OJ(9)         9.68  81.0  26.26 31.38 35.64 39.11 44.43 48.41
      54.85 Primary Thermo Library: MRH (Species ID: C4H7OJ(9))
!     H                 52.1  27.41 4.97  4.97  4.97  4.97  4.97  4.97
      4.97  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009800)
!     C2H5              28.36 59.05 12.11 14.59 17.07 19.35 22.93 25.78
      30.3  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002703)
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 Estimated by Group Additivity
!     C4H7O_1_2         -8.11 80.56 25.48 30.4  34.84 38.6  44.45 48.8
      55.64 Primary Thermo Library: MRH (Species ID: C4H7O_1_2)
!     C4H7-11           58.99 75.0  20.38 25.34 29.68 33.36 39.14 43.48
      50.22 Estimated by Group Additivity
!     OH          9.4   43.91 7.14  7.07  7.05  7.06  7.15  7.34  7.87
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00010102)
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 Estimated by Group Additivity
!     C3H5OJ(13)        4.5   76.14 18.65 22.05 25.01 27.57 32.16 35.43
      39.19 Estimated by Group Additivity
!     C4H7OJ(16)        -0.43 85.56 24.15 29.0  33.26 36.92 43.23 47.77
      53.44 Estimated by Group Additivity
!     CH2CHO            6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34
      26.35 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002559)
!     C4H7OJ(13)        -2.61 86.64 23.05 27.77 32.28 36.23 42.54 47.26
      54.54 Primary Thermo Library: MRH (Species ID: C4H7OJ(13))
!     C3H7-1            23.67 69.29 17.11 21.27 25.14 28.53 33.95 38.14
      44.75 Estimated by Group Additivity
!     HCO         10.04 53.61 8.27  8.72  9.24  9.78  10.74 11.49 12.59
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009325)
!     C4H7OJ(8)         -12.53      83.27 24.09 28.93 33.21 36.9  43.23
      47.78 53.46 Estimated by Group Additivity
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!     C3H8              -24.82      64.56 17.67 22.49 26.86 30.74 37.01
      41.73 48.83 Primary Thermo Library: GRI-Mech3.0 (Species ID:
s00003749)
!     CO          -26.42      47.23 6.96  7.02  7.12  7.27  7.62  7.93
      8.41  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009358)
!Here are the path reactions and their high-P limit kinetics:
!     C4H8O-enol=nC4H8O             8.590e+11    0.32        55900.00
!     CH3+C3H5O-enol2=C4H8O-enol    1.000e+13    0.00        0.00
!     C4H7OJ(9)+H=C4H8O-enol        1.000e+14    0.00        0.00
!     C2H5+C2H3O-1=C4H8O-enol 1.000e+13    0.00        0.00
!     C4H7O_1_2+H=C4H8O-enol        5.000e+13    0.00        0.00
!     C4H7-11+OH=C4H8O-enol   1.000e+13    0.00        0.00
!     C4H7OJ(12)+H=C4H8O-enol       1.000e+13    0.00        0.00
!     CH3+C3H5OJ(13)=nC4H8O         3.370e+13    0.00        0.00
!     C4H7OJ(16)+H=nC4H8O           1.000e+14    0.00        0.00
!     C2H5+CH2CHO=nC4H8O      1.000e+13    0.00        0.00
!     C4H7OJ(13)+H=nC4H8O           2.000e+13    0.00        0.00
!     C3H7-1+HCO=nC4H8O       1.810e+13    0.00        0.00
!     C4H7OJ(12)+H=nC4H8O           5.000e+13    0.00        0.00
!     C4H7OJ(8)+H=nC4H8O            1.000e+13    0.00        0.00
!     C3H8+CO=nC4H8O          9.140e+04    2.53        85500.00

C4H8O-enol(+m)=nC4H8O(+m)                         1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
ReactionLibrary: Tautomerization    deltaHrxn(T=298K) = -
7.18945525056921 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.0685000e+01 2.2888000e-01 -3.3032000e-02 2.0907000e-04 /
CHEB / 1.6820000e+01 4.3045000e-01 -5.8800000e-02 -6.8637000e-04 /
CHEB / -3.9390000e-01 3.5733000e-01 -4.0178000e-02 -3.2348000e-03 /
CHEB / -3.2316000e-01 2.6046000e-01 -1.7788000e-02 -5.5452000e-03 /

CH3+C3H5O-enol2(+m)=nC4H8O(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
83.14609407823946 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0029000e+01 -1.2782000e+00 -1.0749000e-01 5.9138000e-03 /
CHEB / 1.3037000e+00 1.2410000e+00 -1.5772000e-01 5.5270000e-04 /
CHEB / -1.1771000e-01 7.9058000e-01 -4.8657000e-02 -1.4642000e-02 /
CHEB / -3.4980000e-01 3.6571000e-01 2.2697000e-02 -1.5440000e-02 /

CH3+C3H5O-enol2(+m)=C4H8O-enol(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ C_methyl , C_rad/H2/Cd ]
      deltaHrxn(T=298K) = -75.95663882767025 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2655000e+01 4.0902000e-01 -7.9459000e-02 3.7208000e-03 /
CHEB / -7.6727000e-01 7.3332000e-01 -1.2772000e-01 -3.3448000e-04 /
CHEB / -5.8475000e-01 5.3367000e-01 -6.1723000e-02 -1.3196000e-02 /
CHEB / -3.7611000e-01 3.1557000e-01 -3.1154000e-03 -1.8808000e-02 /

C4H7OJ(9)+H(+m)=nC4H8O(+m)                        1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
111.19446182799187 kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1488000e+01 1.4847000e-01 -5.4874000e-01 1.0120000e-01 /
CHEB / -9.6812000e-01 2.1158000e+00 -1.9202000e-01 -3.3273000e-02 /
CHEB / -8.4612000e-01 8.9274000e-01 3.6811000e-02 -3.7927000e-02 /
CHEB / -4.8899000e-01 2.7391000e-01 5.9376000e-02 -1.3989000e-02 /

C4H7OJ(9)+H(+m)=C4H8O-enol(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination exact:  [ C_rad/H2/Cs , H_rad ] deltaHrxn(T=298K) = -
104.00500657742266 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2887000e+01 1.4803000e+00 -4.4690000e-01 1.0329000e-01 /
CHEB / -1.9904000e+00 1.7894000e+00 -2.8507000e-01 -2.9917000e-02 /
CHEB / -1.1088000e+00 8.2898000e-01 1.3084000e-02 -6.0632000e-02 /
CHEB / -5.5646000e-01 2.9455000e-01 7.7799000e-02 -2.8842000e-02 /

C4H7OJ(9)+H(+m)=CH3+C3H5O-enol2(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
28.048367749752423 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3079000e+01 -1.1115000e+00 -1.6197000e-01 2.6813000e-02 /
CHEB / 8.3923000e-01 9.4904000e-01 2.2529000e-02 -4.9260000e-02 /
CHEB / 1.6066000e-01 2.7158000e-01 1.1242000e-01 -1.2439000e-02 /
CHEB / -2.4897000e-02 -1.5998000e-02 5.6016000e-02 2.1269000e-02 /

C2H5+C2H3O-1(+m)=nC4H8O(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
107.26424020628454 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0428000e+01 -1.0450000e-01 -4.6810000e-01 8.6489000e-02 /
CHEB / -6.7339000e-01 2.0532000e+00 -2.0327000e-01 -2.8803000e-02 /
CHEB / -7.8641000e-01 8.9686000e-01 2.6024000e-02 -3.4766000e-02 /
CHEB / -4.8749000e-01 2.8283000e-01 5.7622000e-02 -1.3915000e-02 /

C2H5+C2H3O-1(+m)=C4H8O-enol(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/Cs , Cd_pri_rad ]
      deltaHrxn(T=298K) = -100.07478495571533 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1879000e+01 1.2841000e+00 -3.7034000e-01 8.0876000e-02 /
CHEB / -1.7423000e+00 1.6798000e+00 -2.8447000e-01 -1.6193000e-02 /
CHEB / -1.0584000e+00 8.1800000e-01 -3.6791000e-03 -5.5759000e-02 /
CHEB / -5.5248000e-01 3.0400000e-01 7.1671000e-02 -3.0690000e-02 /

C2H5+C2H3O-1(+m)=CH3+C3H5O-enol2(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
24.11814612804509 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1772000e+01 -1.1674000e+00 -1.4392000e-01 2.3069000e-02 /
CHEB / 1.0878000e+00 9.7275000e-01 -2.8126000e-03 -4.0562000e-02 /
CHEB / 1.8527000e-01 3.0074000e-01 1.0733000e-01 -1.7669000e-02 /
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CHEB / -3.8296000e-02 -7.2495000e-03 6.3612000e-02 1.7402000e-02 /

C4H7OJ(9)+H(+m)=C2H5+C2H3O-1(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -3.930221621707336
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.8997000e+00 -9.9791000e-01 -1.6723000e-01 2.0337000e-02 /
CHEB / 2.6484000e+00 9.5443000e-01 5.7746000e-02 -4.9264000e-02 /
CHEB / 4.6072000e-01 1.7403000e-01 1.1833000e-01 3.5681000e-03 /
CHEB / 1.5112000e-02 -6.1908000e-02 2.9604000e-02 2.6074000e-02 /

C4H7O_1_2+H(+m)=nC4H8O(+m)                      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
93.40634016537044 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1206000e+01 -1.0403000e+00 -1.6518000e-01 1.7413000e-02 /
CHEB / 4.6786000e-01 1.5430000e+00 -2.0167000e-01 5.0480000e-04 /
CHEB / -3.8945000e-01 8.6264000e-01 -3.0287000e-02 -2.3228000e-02 /
CHEB / -4.0788000e-01 3.3996000e-01 4.1311000e-02 -1.6200000e-02 /

C4H7O_1_2+H(+m)=C4H8O-enol(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H/OneDeC , H_rad ]
      deltaHrxn(T=298K) = -86.21688491480123 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3235000e+01 6.0023000e-01 -1.3051000e-01 1.3491000e-02 /
CHEB / -1.1028000e+00 1.0181000e+00 -1.8402000e-01 2.6161000e-03 /
CHEB / -7.5348000e-01 6.6059000e-01 -6.0413000e-02 -2.3490000e-02 /
CHEB / -4.5194000e-01 3.3350000e-01 2.0710000e-02 -2.7061000e-02 /

C4H7O_1_2+H(+m)=CH3+C3H5O-enol2(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
10.260246087130996 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1254000e+01 -1.3793000e+00 -8.2270000e-02 5.8565000e-03 /
CHEB / 2.2307000e+00 9.6058000e-01 -7.1757000e-02 -1.0606000e-02 /
CHEB / 3.4977000e-01 4.4666000e-01 5.0365000e-02 -2.1908000e-02 /
CHEB / -7.9214000e-02 8.0215000e-02 7.7895000e-02 -4.5193000e-03 /

C4H7OJ(9)+H(+m)=C4H7O_1_2+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
17.788121662621435 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0239000e+01 -1.0886000e+00 -1.5870000e-01 2.4191000e-02 /
CHEB / 1.8913000e+00 9.6244000e-01 2.8201000e-02 -4.7859000e-02 /
CHEB / 4.1510000e-01 2.4817000e-01 1.1427000e-01 -8.3011000e-03 /
CHEB / 3.5263000e-02 -3.3925000e-02 4.9659000e-02 2.2942000e-02 /

C4H7O_1_2+H(+m)=C2H5+C2H3O-1(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = 13.857900040914092
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 4    4 /
CHEB / 6.1438000e+00 -1.1385000e+00 -1.4299000e-01 2.1188000e-02 /
CHEB / 6.0629000e+00 9.8680000e-01 5.1046000e-03 -4.0582000e-02 /
CHEB / 2.6739000e-01 2.7369000e-01 1.1147000e-01 -1.3440000e-02 /
CHEB / -2.9649000e-02 -2.7964000e-02 5.7116000e-02 2.0209000e-02 /

C4H7-11+OH(+m)=nC4H8O(+m)                       1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
117.8099357056716 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7425000e+00 1.1916000e+00 -8.6614000e-01 1.5958000e-01 /
CHEB / -1.3524000e+00 2.2383000e+00 -1.1698000e-01 -7.5264000e-02 /
CHEB / -1.0036000e+00 8.5636000e-01 7.8382000e-02 -4.7598000e-02 /
CHEB / -5.3139000e-01 2.4622000e-01 6.5155000e-02 -1.3144000e-02 /

C4H7-11+OH(+m)=C4H8O-enol(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ Cd_pri_rad , O_pri_rad ]
      deltaHrxn(T=298K) = -110.6204804551024 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1016000e+01 2.3620000e+00 -7.8565000e-01 1.8496000e-01 /
CHEB / -2.2611000e+00 2.0529000e+00 -2.0710000e-01 -1.0359000e-01 /
CHEB / -1.2446000e+00 8.2976000e-01 7.4563000e-02 -6.9427000e-02 /
CHEB / -6.0632000e-01 2.6081000e-01 9.0213000e-02 -2.1019000e-02 /

C4H7-11+OH(+m)=CH3+C3H5O-enol2(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
34.663841627432156 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2253000e+01 -8.9471000e-01 -2.1956000e-01 2.5298000e-02 /
CHEB / 6.4549000e-01 8.1320000e-01 1.1752000e-01 -6.3102000e-02 /
CHEB / 1.0291000e-01 1.8726000e-01 1.0917000e-01 1.1671000e-02 /
CHEB / -2.7316000e-02 -3.2917000e-02 2.8498000e-02 2.6070000e-02 /

C4H7OJ(9)+H(+m)=C4H7-11+OH(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = 6.6154738776797295
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.0475000e+00 -8.4111000e-01 -1.9934000e-01 1.5513000e-02 /
CHEB / 4.6676000e+00 8.4187000e-01 1.2318000e-01 -5.1410000e-02 /
CHEB / 5.0760000e-01 1.1606000e-01 1.0232000e-01 2.0444000e-02 /
CHEB / 5.5933000e-02 -6.6465000e-02 8.3846000e-03 2.3151000e-02 /

C4H7-11+OH(+m)=C2H5+C2H3O-1(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -10.545695499387069
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.6876000e+00 -8.5423000e-01 -1.9993000e-01 1.6969000e-02 /
CHEB / 1.9096000e+00 8.4489000e-01 1.2018000e-01 -5.2802000e-02 /
CHEB / 4.2795000e-01 1.2726000e-01 1.0354000e-01 1.8959000e-02 /
CHEB / 2.8968000e-02 -6.4253000e-02 1.1357000e-02 2.3707000e-02 /
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C4H7-11+OH(+m)=C4H7O_1_2+H(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -24.40359554030117
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.5851000e+00 -8.9191000e-01 -2.1057000e-01 2.2952000e-02 /
CHEB / 1.5718000e+00 8.3027000e-01 1.1510000e-01 -5.9423000e-02 /
CHEB / 3.4756000e-01 1.7396000e-01 1.0725000e-01 1.3203000e-02 /
CHEB / 3.7485000e-02 -4.4106000e-02 2.3960000e-02 2.5329000e-02 /

C4H7OJ(12)+H(+m)=nC4H8O(+m)                       1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H/OneDeC , H_rad ]
      deltaHrxn(T=298K) = -95.17652384996701 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3122000e+01 5.3966000e-01 -9.3484000e-02 1.2189000e-02 /
CHEB / -1.1327000e+00 8.5072000e-01 -1.0114000e-01 -1.0829000e-03 /
CHEB / -7.5578000e-01 4.8391000e-01 -1.0311000e-02 -1.0955000e-02 /
CHEB / -4.4010000e-01 2.0538000e-01 2.2781000e-02 -4.4860000e-03 /

C4H7OJ(12)+H(+m)=C4H8O-enol(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ O_rad/OneDe , H_rad ]
      deltaHrxn(T=298K) = -87.9870685993978 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2499000e+01 5.5546000e-01 -1.0714000e-01 7.9102000e-03 /
CHEB / -1.0274000e+00 9.5176000e-01 -1.5158000e-01 -2.4275000e-03 /
CHEB / -7.2776000e-01 6.1495000e-01 -4.0181000e-02 -2.4432000e-02 /
CHEB / -4.4523000e-01 3.0335000e-01 3.0893000e-02 -2.4621000e-02 /

C4H7OJ(12)+H(+m)=CH3+C3H5O-enol2(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
12.030429771727563 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0718000e+01 -1.3747000e+00 -8.1684000e-02 5.6644000e-03 /
CHEB / 2.0817000e+00 9.6901000e-01 -7.1663000e-02 -1.0461000e-02 /
CHEB / 3.2736000e-01 4.4346000e-01 5.3067000e-02 -2.2165000e-02 /
CHEB / -8.4344000e-02 7.3039000e-02 7.8729000e-02 -3.5840000e-03 /

C4H7OJ(9)+H(+m)=C4H7OJ(12)+H(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
16.01793797802486 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.0285000e+00 -1.0853000e+00 -1.5845000e-01 2.4035000e-02 /
CHEB / 1.8979000e+00 9.6632000e-01 2.9241000e-02 -4.8049000e-02 /
CHEB / 4.1530000e-01 2.4358000e-01 1.1515000e-01 -7.5432000e-03 /
CHEB / 3.0466000e-02 -3.7526000e-02 4.8403000e-02 2.3412000e-02 /

C4H7OJ(12)+H(+m)=C2H5+C2H3O-1(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = 12.087716356317525
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
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CHEB / 5.8317000e+00 -1.1347000e+00 -1.4298000e-01 2.1215000e-02 /
CHEB / 5.6601000e+00 9.9109000e-01 6.2756000e-03 -4.1031000e-02 /
CHEB / 3.0140000e-01 2.6862000e-01 1.1279000e-01 -1.2739000e-02 /
CHEB / -3.4340000e-02 -3.2021000e-02 5.5875000e-02 2.0895000e-02 /

C4H7OJ(12)+H(+m)=C4H7O_1_2+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
1.7701836845965673 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.3578000e+00 -1.3196000e+00 -9.0482000e-02 7.6323000e-03 /
CHEB / 3.6152000e+00 1.0045000e+00 -6.1490000e-02 -1.4356000e-02 /
CHEB / 5.3057000e-01 4.0064000e-01 7.3712000e-02 -2.2633000e-02 /
CHEB / -3.6081000e-02 2.9829000e-02 7.9409000e-02 2.8960000e-03 /

C4H7-11+OH(+m)=C4H7OJ(12)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -22.633411855704594
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.4164000e+00 -8.9148000e-01 -2.0929000e-01 2.2536000e-02 /
CHEB / 1.5430000e+00 8.3429000e-01 1.1496000e-01 -5.8911000e-02 /
CHEB / 3.4738000e-01 1.7096000e-01 1.0724000e-01 1.3626000e-02 /
CHEB / 3.4419000e-02 -4.6534000e-02 2.2974000e-02 2.5284000e-02 /

CH3+C3H5OJ(13)(+m)=nC4H8O(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination exact:  [ C_methyl , C_rad/H2/Cs ]    deltaHrxn(T=298K)
= -89.02538476147296 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3144000e+01 4.1966000e-01 -5.9562000e-02 3.7390000e-03 /
CHEB / -1.0004000e+00 7.1319000e-01 -7.9831000e-02 -1.4016000e-03 /
CHEB / -6.7884000e-01 4.5079000e-01 -1.5166000e-02 -9.5227000e-03 /
CHEB / -3.9909000e-01 2.1300000e-01 2.0671000e-02 -6.9466000e-03 /

CH3+C3H5OJ(13)(+m)=C4H8O-enol(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
81.83592951090375 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0181000e+01 -1.0988000e+00 -1.3479000e-01 1.1221000e-02 /
CHEB / 6.7505000e-01 1.4771000e+00 -1.6956000e-01 -1.0835000e-03 /
CHEB / -3.5079000e-01 8.4346000e-01 -2.0453000e-02 -2.0337000e-02 /
CHEB / -4.2186000e-01 3.3445000e-01 4.4792000e-02 -1.3994000e-02 /

CH3+C3H5O-enol2(+m)=CH3+C3H5OJ(13)(+m)          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
5.879290683233508 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.5133000e+00 -2.6695000e+00 -1.5604000e-01 9.7252000e-03 /
CHEB / 5.4519000e+00 1.9169000e+00 -1.0421000e-01 -2.2161000e-02 /
CHEB / 2.0660000e-01 7.4049000e-01 9.7309000e-02 -2.6353000e-02 /
CHEB / -2.5822000e-01 8.4833000e-02 9.4809000e-02 7.4118000e-04 /
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C4H7OJ(9)+H(+m)=CH3+C3H5OJ(13)(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
22.169077066518916 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1242000e+01 -1.8002000e+00 -3.5741000e-01 3.0073000e-02 /
CHEB / 1.4071000e+00 1.6414000e+00 1.8107000e-01 -7.5740000e-02 /
CHEB / 1.0559000e-01 3.4203000e-01 1.6556000e-01 6.0112000e-03 /
CHEB / -1.0703000e-01 -7.1524000e-02 4.6786000e-02 2.6232000e-02 /

C2H5+C2H3O-1(+m)=CH3+C3H5OJ(13)(+m)       1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -18.238855444811584
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.8998000e+00 -1.9363000e+00 -3.2944000e-01 3.2551000e-02 /
CHEB / 1.7268000e+00 1.7376000e+00 1.3507000e-01 -7.4371000e-02 /
CHEB / 1.2586000e-01 3.8314000e-01 1.6809000e-01 2.8587000e-04 /
CHEB / -1.2884000e-01 -6.6604000e-02 5.6780000e-02 2.3748000e-02 /

C4H7O_1_2+H(+m)=CH3+C3H5OJ(13)(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
4.380955403897486 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.9184000e+00 -2.5057000e+00 -1.8652000e-01 1.5380000e-02 /
CHEB / 3.6122000e+00 1.9701000e+00 -6.7534000e-02 -3.3759000e-02 /
CHEB / 2.1372000e-01 6.3646000e-01 1.3393000e-01 -2.3844000e-02 /
CHEB / -2.2131000e-01 1.6423000e-02 9.2680000e-02 8.1422000e-03 /

C4H7-11+OH(+m)=CH3+C3H5OJ(13)(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -28.78455094419865
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0473000e+01 -1.3325000e+00 -4.1184000e-01 1.4710000e-03 /
CHEB / 1.0522000e+00 1.2662000e+00 2.9977000e-01 -5.4578000e-02 /
CHEB / 5.7609000e-02 2.2673000e-01 1.4041000e-01 2.7317000e-02 /
CHEB / -8.6706000e-02 -7.2460000e-02 1.5173000e-02 2.7101000e-02 /

C4H7OJ(12)+H(+m)=CH3+C3H5OJ(13)(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
6.1511390884940536 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1047000e+01 -1.1882000e+00 -9.9621000e-02 1.0016000e-02 /
CHEB / 2.1186000e+00 1.0308000e+00 -1.4075000e-02 -2.1343000e-02 /
CHEB / 2.2651000e-01 2.9107000e-01 8.8290000e-02 -9.0225000e-03 /
CHEB / -9.5336000e-02 -3.6384000e-02 4.7216000e-02 1.2117000e-02 /

C4H7OJ(16)+H(+m)=nC4H8O(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination exact:  [ C_rad/H2/Cs , H_rad ] deltaHrxn(T=298K) = -
101.08568581165667 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3062000e+01 8.9684000e-01 -2.0966000e-01 4.4030000e-02 /
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CHEB / -1.4317000e+00 1.0713000e+00 -8.2961000e-02 -2.9381000e-02 /
CHEB / -8.9090000e-01 5.0018000e-01 3.2546000e-02 -1.9419000e-02 /
CHEB / -4.6943000e-01 1.7153000e-01 4.0936000e-02 4.4839000e-04 /

C4H7OJ(16)+H(+m)=C4H8O-enol(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
93.89623056108746 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0764000e+01 -5.4624000e-01 -3.0609000e-01 5.4823000e-02 /
CHEB / -2.3563000e-01 1.8761000e+00 -1.7927000e-01 -2.7819000e-02 /
CHEB / -6.6529000e-01 8.6092000e-01 3.1200000e-02 -3.0868000e-02 /
CHEB / -4.8377000e-01 2.7823000e-01 6.0578000e-02 -9.9903000e-03 /

C4H7OJ(16)+H(+m)=CH3+C3H5O-enol2(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
17.939591733417224 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.4369000e+00 -2.3333000e+00 -2.4287000e-01 2.8330000e-02 /
CHEB / 2.3017000e+00 1.8991000e+00 -1.2761000e-03 -5.5013000e-02 /
CHEB / 1.7926000e-01 5.5203000e-01 1.5065000e-01 -1.7297000e-02 /
CHEB / -1.6511000e-01 -6.4781000e-03 8.2062000e-02 1.3199000e-02 /

C4H7OJ(9)+H(+m)=C4H7OJ(16)+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
10.108776016335199 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.1742000e+00 -1.6859000e+00 -3.4645000e-01 1.8187000e-02 /
CHEB / 2.8111000e+00 1.6161000e+00 2.0105000e-01 -6.4381000e-02 /
CHEB / 3.9427000e-01 2.5706000e-01 1.5528000e-01 1.6268000e-02 /
CHEB / -3.2070000e-02 -9.5825000e-02 2.9154000e-02 2.5121000e-02 /

C4H7OJ(16)+H(+m)=C2H5+C2H3O-1(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = 6.178554394627863
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.2316000e+00 -1.7937000e+00 -3.2856000e-01 2.1483000e-02 /
CHEB / 4.8536000e+00 1.7010000e+00 1.6704000e-01 -6.5812000e-02 /
CHEB / 2.9524000e-01 2.8428000e-01 1.6207000e-01 1.1931000e-02 /
CHEB / -8.5416000e-02 -9.4320000e-02 3.6703000e-02 2.4512000e-02 /

C4H7OJ(16)+H(+m)=C4H7O_1_2+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
7.6793456462862295 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.2940000e+00 -2.2124000e+00 -2.5481000e-01 2.6080000e-02 /
CHEB / 3.5259000e+00 1.9098000e+00 3.0490000e-02 -5.7568000e-02 /
CHEB / 3.9544000e-01 4.6903000e-01 1.6366000e-01 -9.8795000e-03 /
CHEB / -1.0385000e-01 -4.8740000e-02 7.1485000e-02 1.7903000e-02 /

C4H7-11+OH(+m)=C4H7OJ(16)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -16.724249894014932
kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.6719000e+00 -1.2955000e+00 -3.8360000e-01 -5.4852000e-03 /
CHEB / 2.2491000e+00 1.2752000e+00 2.9217000e-01 -4.2141000e-02 /
CHEB / 3.5176000e-01 1.8056000e-01 1.2530000e-01 2.9247000e-02 /
CHEB / -7.2737000e-03 -8.8460000e-02 5.3365000e-03 2.2858000e-02 /

C4H7OJ(12)+H(+m)=C4H7OJ(16)+H(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
5.909161961689662 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.1043000e+00 -9.9165000e-01 -1.4854000e-01 1.6883000e-02 /
CHEB / 4.4474000e+00 9.5795000e-01 6.0019000e-02 -3.9233000e-02 /
CHEB / 4.0309000e-01 1.6939000e-01 9.8765000e-02 5.6697000e-03 /
CHEB / -6.2930000e-03 -6.9913000e-02 2.0932000e-02 1.7906000e-02 /

C4H7OJ(16)+H(+m)=CH3+C3H5OJ(13)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
12.060301050183716 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1988000e+01 -1.0291000e+00 -1.4621000e-01 1.9200000e-02 /
CHEB / 1.4476000e+00 9.6822000e-01 4.8711000e-02 -4.0075000e-02 /
CHEB / 2.0069000e-01 1.9909000e-01 1.0085000e-01 1.2258000e-03 /
CHEB / -4.7864000e-02 -6.3055000e-02 2.8919000e-02 1.8296000e-02 /

C2H5+CH2CHO(+m)=nC4H8O(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O) High-P Limit: R_Recombination estimate:
(Average:) [ C_rad/H2/Cs , C_rad/H2/CO ]  deltaHrxn(T=298K) = -
83.77365543639377 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2794000e+01 3.1880000e-01 -3.9285000e-02 5.6099000e-04 /
CHEB / -8.6650000e-01 5.6536000e-01 -5.9611000e-02 -1.9138000e-03 /
CHEB / -5.6845000e-01 3.9472000e-01 -2.0567000e-02 -6.1673000e-03 /
CHEB / -3.7098000e-01 2.1463000e-01 9.4124000e-03 -6.0428000e-03 /

C2H5+CH2CHO(+m)=C4H8O-enol(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -76.58420018582456
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.4446000e+00 -1.2349000e+00 -1.0463000e-01 5.7398000e-03 /
CHEB / 1.1120000e+00 1.3024000e+00 -1.4698000e-01 -5.4818000e-04 /
CHEB / -1.7991000e-01 8.0595000e-01 -3.3597000e-02 -1.5135000e-02 /
CHEB / -4.0397000e-01 3.5448000e-01 3.2996000e-02 -1.3809000e-02 /

CH3+C3H5O-enol2(+m)=C2H5+CH2CHO(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
0.6275613581543116 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.3800000e+00 -2.7640000e+00 -1.3915000e-01 6.2775000e-03 /
CHEB / 4.5827000e+00 1.8653000e+00 -1.1972000e-01 -1.6213000e-02 /
CHEB / 2.1177000e-01 7.9771000e-01 7.1628000e-02 -2.5659000e-02 /
CHEB / -2.9524000e-01 1.3186000e-01 9.2054000e-02 -3.6437000e-03 /
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C4H7OJ(9)+H(+m)=C2H5+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -27.420806391598113
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1647000e+01 -1.8358000e+00 -3.6372000e-01 3.4568000e-02 /
CHEB / 9.5788000e-01 1.6428000e+00 1.7342000e-01 -7.9803000e-02 /
CHEB / -3.5568000e-03 3.7149000e-01 1.7000000e-01 1.0003000e-03 /
CHEB / -1.3641000e-01 -5.8443000e-02 5.4381000e-02 2.6062000e-02 /

C2H5+C2H3O-1(+m)=C2H5+CH2CHO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -23.49058476989078
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0338000e+01 -1.9810000e+00 -3.3235000e-01 3.6471000e-02 /
CHEB / 1.2544000e+00 1.7396000e+00 1.2368000e-01 -7.6985000e-02 /
CHEB / 1.7097000e-02 4.1818000e-01 1.7000000e-01 -5.0997000e-03 /
CHEB / -1.5769000e-01 -5.0970000e-02 6.4913000e-02 2.2559000e-02 /

C4H7O_1_2+H(+m)=C2H5+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -9.632684728976683
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.6050000e+00 -2.5898000e+00 -1.7259000e-01 1.3175000e-02 /
CHEB / 2.9296000e+00 1.9464000e+00 -8.7885000e-02 -2.8408000e-02 /
CHEB / 1.4958000e-01 6.9520000e-01 1.1609000e-01 -2.6333000e-02 /
CHEB / -2.5108000e-01 5.3207000e-02 9.6017000e-02 3.7451000e-03 /

C4H7-11+OH(+m)=C2H5+CH2CHO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -34.036280269277846
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0781000e+01 -1.3400000e+00 -4.2517000e-01 4.8634000e-03 /
CHEB / 6.6484000e-01 1.2595000e+00 3.0400000e-01 -6.1016000e-02 /
CHEB / -4.8627000e-02 2.4142000e-01 1.4756000e-01 2.6510000e-02 /
CHEB / -1.1764000e-01 -6.5152000e-02 1.9773000e-02 2.9253000e-02 /

C4H7OJ(12)+H(+m)=C2H5+CH2CHO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -11.40286841357325
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1743000e+01 -1.2382000e+00 -9.1051000e-02 8.8190000e-03 /
CHEB / 1.4067000e+00 1.0204000e+00 -2.6603000e-02 -1.7939000e-02 /
CHEB / 1.1913000e-01 3.3359000e-01 7.8195000e-02 -1.1225000e-02 /
CHEB / -1.2487000e-01 -1.1355000e-02 5.2565000e-02 9.0018000e-03 /

CH3+C3H5OJ(13)(+m)=C2H5+CH2CHO(+m)        1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -5.251729325079195
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1081000e+01 -1.3070000e+00 -7.3742000e-02 4.5053000e-03 /
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CHEB / 1.9251000e+00 1.0136000e+00 -4.5117000e-02 -1.0943000e-02 /
CHEB / 1.4589000e-01 3.8882000e-01 6.2399000e-02 -1.2720000e-02 /
CHEB / -1.3830000e-01 1.7619000e-02 5.8797000e-02 4.5810000e-03 /

C4H7OJ(16)+H(+m)=C2H5+CH2CHO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -17.312030375262914
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2541000e+01 -1.0662000e+00 -1.4358000e-01 2.0650000e-02 /
CHEB / 8.6602000e-01 9.6749000e-01 3.8523000e-02 -3.9783000e-02 /
CHEB / 7.4443000e-02 2.3127000e-01 9.8792000e-02 -2.4334000e-03 /
CHEB / -7.8365000e-02 -4.8586000e-02 3.5864000e-02 1.7111000e-02 /

C4H7OJ(13)+H(+m)=nC4H8O(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination exact:  [ C_rad/H/NonDeC , H_rad ]    deltaHrxn(T=298K)
= -98.90612557528924 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2637000e+01 7.3769000e-01 -1.5299000e-01 2.7882000e-02 /
CHEB / -1.4197000e+00 1.0054000e+00 -9.8424000e-02 -1.5394000e-02 /
CHEB / -8.4535000e-01 5.0064000e-01 1.8705000e-02 -1.8632000e-02 /
CHEB / -4.6472000e-01 1.8288000e-01 3.8849000e-02 -2.6008000e-03 /

C4H7OJ(13)+H(+m)=C4H8O-enol(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
91.71667032472003 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0205000e+01 -7.1643000e-01 -2.4782000e-01 3.9412000e-02 /
CHEB / -1.3237000e-01 1.7988000e+00 -1.8927000e-01 -1.6668000e-02 /
CHEB / -5.9860000e-01 8.6432000e-01 1.8926000e-02 -2.9840000e-02 /
CHEB / -4.7950000e-01 2.9051000e-01 5.8729000e-02 -1.0875000e-02 /

C4H7OJ(13)+H(+m)=CH3+C3H5O-enol2(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
15.76003149704979 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.6220000e+00 -2.4297000e+00 -2.1574000e-01 2.3070000e-02 /
CHEB / 2.4845000e+00 1.9291000e+00 -3.6336000e-02 -4.5135000e-02 /
CHEB / 2.0469000e-01 5.9852000e-01 1.4160000e-01 -2.1320000e-02 /
CHEB / -1.8799000e-01 1.0680000e-02 8.7426000e-02 1.0321000e-02 /

C4H7OJ(9)+H(+m)=C4H7OJ(13)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
12.288336252702635 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.1843000e+00 -1.7174000e+00 -3.4827000e-01 2.1128000e-02 /
CHEB / 2.4920000e+00 1.6267000e+00 1.9575000e-01 -6.7289000e-02 /
CHEB / 3.3672000e-01 2.7853000e-01 1.5778000e-01 1.4066000e-02 /
CHEB / -4.6600000e-02 -9.1533000e-02 3.3313000e-02 2.5531000e-02 /
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C4H7OJ(13)+H(+m)=C2H5+C2H3O-1(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = 8.3581146309953
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.1768000e+00 -1.8330000e+00 -3.2767000e-01 2.4291000e-02 /
CHEB / 5.2684000e+00 1.7160000e+00 1.5836000e-01 -6.8145000e-02 /
CHEB / 2.6529000e-01 3.0881000e-01 1.6388000e-01 9.3609000e-03 /
CHEB / -1.0065000e-01 -8.9626000e-02 4.1562000e-02 2.4550000e-02 /

C4H7O_1_2+H(+m)=C4H7OJ(13)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
5.499785409918793 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.2729000e+00 -2.2958000e+00 -2.3368000e-01 2.3157000e-02 /
CHEB / 5.2497000e+00 1.9449000e+00 -6.1881000e-04 -5.0794000e-02 /
CHEB / 3.1985000e-01 5.0840000e-01 1.5999000e-01 -1.4430000e-02 /
CHEB / -1.4420000e-01 -3.7175000e-02 7.7848000e-02 1.5922000e-02 /

C4H7-11+OH(+m)=C4H7OJ(13)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -18.903810130382368
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.6146000e+00 -1.3069000e+00 -3.8979000e-01 -3.9113000e-03 /
CHEB / 1.9873000e+00 1.2748000e+00 2.9364000e-01 -4.4818000e-02 /
CHEB / 2.9047000e-01 1.9277000e-01 1.2867000e-01 2.8764000e-02 /
CHEB / -2.2830000e-02 -8.5163000e-02 7.5420000e-03 2.3775000e-02 /

C4H7OJ(12)+H(+m)=C4H7OJ(13)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
3.729601725322226 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.3351000e+00 -1.0509000e+00 -1.3260000e-01 1.5091000e-02 /
CHEB / 3.8831000e+00 9.9428000e-01 3.4797000e-02 -3.4027000e-02 /
CHEB / 3.8352000e-01 1.9662000e-01 1.0025000e-01 5.4169000e-04 /
CHEB / -2.5489000e-02 -6.6264000e-02 2.8309000e-02 1.7298000e-02 /

C4H7OJ(13)+H(+m)=CH3+C3H5OJ(13)(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
9.88074081381628 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1188000e+01 -1.0965000e+00 -1.2612000e-01 1.5787000e-02 /
CHEB / 1.5818000e+00 1.0063000e+00 1.9455000e-02 -3.2378000e-02 /
CHEB / 2.1450000e-01 2.3196000e-01 9.9830000e-02 -4.2233000e-03 /
CHEB / -6.7858000e-02 -5.7378000e-02 3.7407000e-02 1.6573000e-02 /

C4H7OJ(16)+H(+m)=C4H7OJ(13)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
2.1795602363674362 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.5847000e+00 -9.3007000e-01 -1.5966000e-01 1.6327000e-02 /
CHEB / 2.8884000e+00 9.3487000e-01 8.0338000e-02 -4.1391000e-02 /
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CHEB / 4.3127000e-01 1.2859000e-01 1.0022000e-01 1.0322000e-02 /
CHEB / 1.1172000e-02 -7.8811000e-02 1.1926000e-02 1.9031000e-02 /

C4H7OJ(13)+H(+m)=C2H5+CH2CHO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -15.132470138895476
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1792000e+01 -1.1397000e+00 -1.2059000e-01 1.6034000e-02 /
CHEB / 9.5559000e-01 1.0037000e+00 7.2865000e-03 -3.0432000e-02 /
CHEB / 9.2269000e-02 2.6889000e-01 9.4806000e-02 -7.6385000e-03 /
CHEB / -9.7655000e-02 -3.9412000e-02 4.4375000e-02 1.4458000e-02 /

C3H7-1+HCO(+m)=nC4H8O(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O) High-P Limit: R_Recombination exact:  [
C_rad/H2/Cs , CO_pri_rad ]    deltaHrxn(T=298K) = -83.12751689722805
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2926000e+01 3.1136000e-01 -3.7974000e-02 4.0510000e-04 /
CHEB / -7.5242000e-01 5.5366000e-01 -5.8040000e-02 -1.9771000e-03 /
CHEB / -5.5860000e-01 3.8936000e-01 -2.0711000e-02 -5.9700000e-03 /
CHEB / -3.6875000e-01 2.1411000e-01 8.5720000e-03 -5.9295000e-03 /

C3H7-1+HCO(+m)=C4H8O-enol(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -75.93806164665884
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.5377000e+00 -1.2452000e+00 -1.0257000e-01 5.4254000e-03 /
CHEB / 1.2565000e+00 1.2880000e+00 -1.4510000e-01 -5.7065000e-04 /
CHEB / -1.6407000e-01 8.0198000e-01 -3.4414000e-02 -1.4760000e-02 /
CHEB / -4.0280000e-01 3.5586000e-01 3.1944000e-02 -1.3735000e-02 /

CH3+C3H5O-enol2(+m)=C3H7-1+HCO(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
0.018577181011394828 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.6757000e+00 -2.7715000e+00 -1.3803000e-01 6.0735000e-03 /
CHEB / 4.6100000e+00 1.8601000e+00 -1.2068000e-01 -1.5837000e-02 /
CHEB / 2.3325000e-01 8.0181000e-01 6.9514000e-02 -2.5553000e-02 /
CHEB / -2.9159000e-01 1.3597000e-01 9.1627000e-02 -3.9770000e-03 /

C4H7OJ(9)+H(+m)=C3H7-1+HCO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -28.066944930763814
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1904000e+01 -1.8387000e+00 -3.6430000e-01 3.4946000e-02 /
CHEB / 1.0191000e+00 1.6429000e+00 1.7274000e-01 -8.0141000e-02 /
CHEB / 8.7774000e-03 3.7390000e-01 1.7040000e-01 5.4006000e-04 /
CHEB / -1.3260000e-01 -5.7274000e-02 5.5060000e-02 2.6024000e-02 /

C2H5+C2H3O-1(+m)=C3H7-1+HCO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -24.13672330905648
kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0598000e+01 -1.9846000e+00 -3.3265000e-01 3.6793000e-02 /
CHEB / 1.3139000e+00 1.7397000e+00 1.2269000e-01 -7.7190000e-02 /
CHEB / 2.9420000e-02 4.2105000e-01 1.7016000e-01 -5.5840000e-03 /
CHEB / -1.5384000e-01 -4.9555000e-02 6.5624000e-02 2.2425000e-02 /

C4H7O_1_2+H(+m)=C3H7-1+HCO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -10.27882326814239
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.8850000e+00 -2.5965000e+00 -1.7165000e-01 1.3034000e-02 /
CHEB / 2.9730000e+00 1.9437000e+00 -8.9353000e-02 -2.8032000e-02 /
CHEB / 1.6507000e-01 6.9976000e-01 1.1454000e-01 -2.6501000e-02 /
CHEB / -2.4704000e-01 5.6537000e-02 9.6155000e-02 3.3726000e-03 /

C4H7-11+OH(+m)=C3H7-1+HCO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -34.68241880844354
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1030000e+01 -1.3405000e+00 -4.2638000e-01 5.1829000e-03 /
CHEB / 7.3092000e-01 1.2589000e+00 3.0440000e-01 -6.1627000e-02 /
CHEB / -3.5970000e-02 2.4258000e-01 1.4822000e-01 2.6434000e-02 /
CHEB / -1.1395000e-01 -6.4523000e-02 2.0194000e-02 2.9454000e-02 /

C4H7OJ(12)+H(+m)=C3H7-1+HCO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -12.049006952738956
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2023000e+01 -1.2421000e+00 -9.0489000e-02 8.7477000e-03 /
CHEB / 1.4483000e+00 1.0191000e+00 -2.7466000e-02 -1.7710000e-02 /
CHEB / 1.3073000e-01 3.3684000e-01 7.7332000e-02 -1.1371000e-02 /
CHEB / -1.2106000e-01 -9.0429000e-03 5.2885000e-02 8.7459000e-03 /

CH3+C3H5OJ(13)(+m)=C3H7-1+HCO(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -5.897867864244901
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1372000e+01 -1.3112000e+00 -7.3073000e-02 4.3833000e-03 /
CHEB / 1.9559000e+00 1.0113000e+00 -4.5791000e-02 -1.0713000e-02 /
CHEB / 1.5979000e-01 3.9225000e-01 6.1167000e-02 -1.2728000e-02 /
CHEB / -1.3443000e-01 2.0626000e-02 5.8853000e-02 4.2919000e-03 /

C4H7OJ(16)+H(+m)=C3H7-1+HCO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -17.95816891442862
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2810000e+01 -1.0691000e+00 -1.4345000e-01 2.0774000e-02 /
CHEB / 9.1734000e-01 9.6711000e-01 3.7766000e-02 -3.9769000e-02 /
CHEB / 8.5018000e-02 2.3379000e-01 9.8594000e-02 -2.7235000e-03 /
CHEB / -7.4764000e-02 -4.7232000e-02 3.6399000e-02 1.6995000e-02 /
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C2H5+CH2CHO(+m)=C3H7-1+HCO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -0.6461385391657046
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0170000e+01 -1.3707000e+00 -6.1795000e-02 1.9370000e-03 /
CHEB / 2.6795000e+00 9.7659000e-01 -5.3718000e-02 -7.2864000e-03 /
CHEB / 1.8703000e-01 4.3790000e-01 4.2337000e-02 -1.1614000e-02 /
CHEB / -1.7709000e-01 6.2480000e-02 5.7327000e-02 5.7240000e-04 /

C4H7OJ(13)+H(+m)=C3H7-1+HCO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -15.778608678061183
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2065000e+01 -1.1430000e+00 -1.2024000e-01 1.6065000e-02 /
CHEB / 1.0036000e+00 1.0031000e+00 6.3995000e-03 -3.0295000e-02 /
CHEB / 1.0301000e-01 2.7177000e-01 9.4356000e-02 -7.8975000e-03 /
CHEB / -9.3978000e-02 -3.7730000e-02 4.4883000e-02 1.4270000e-02 /

C4H7OJ(8)+H(+m)=nC4H8O(+m)                        1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) High-P Limit:
R_Recombination estimate: (Average:) [ CO_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -88.98691183758515 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2612000e+01 3.9819000e-01 -5.4839000e-02 2.8779000e-03 /
CHEB / -9.4593000e-01 6.8365000e-01 -7.5830000e-02 -1.4055000e-03 /
CHEB / -6.5656000e-01 4.4131000e-01 -1.6818000e-02 -8.7205000e-03 /
CHEB / -3.9851000e-01 2.1437000e-01 1.8396000e-02 -6.8729000e-03 /

C4H7OJ(8)+H(+m)=C4H8O-enol(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
81.79745658701594 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.5834000e+00 -1.1272000e+00 -1.2802000e-01 9.8607000e-03 /
CHEB / 7.8050000e-01 1.4431000e+00 -1.6532000e-01 -8.0119000e-04 /
CHEB / -3.1827000e-01 8.3771000e-01 -2.3485000e-02 -1.9246000e-02 /
CHEB / -4.2290000e-01 3.3869000e-01 4.2686000e-02 -1.4073000e-02 /

C4H7OJ(8)+H(+m)=CH3+C3H5O-enol2(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
5.840817759345699 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.9667000e+00 -2.6888000e+00 -1.5222000e-01 8.8986000e-03 /
CHEB / 3.9633000e+00 1.9087000e+00 -1.0790000e-01 -2.0768000e-02 /
CHEB / 2.9453000e-01 7.5262000e-01 9.2343000e-02 -2.6327000e-02 /
CHEB / -2.4423000e-01 9.3533000e-02 9.4624000e-02 -1.5497000e-04 /

C4H7OJ(9)+H(+m)=C4H7OJ(8)+H(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
22.20754999040672 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.0340000e+00 -1.8073000e+00 -3.5854000e-01 3.0938000e-02 /
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CHEB / 1.8991000e+00 1.6418000e+00 1.7964000e-01 -7.6530000e-02 /
CHEB / 2.1296000e-01 3.4784000e-01 1.6638000e-01 5.1063000e-03 /
CHEB / -7.4812000e-02 -6.9134000e-02 4.8189000e-02 2.6236000e-02 /

C2H5+C2H3O-1(+m)=C4H7OJ(8)+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -18.2773283686994
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.6985000e+00 -1.9452000e+00 -3.2991000e-01 3.3319000e-02 /
CHEB / 2.2141000e+00 1.7383000e+00 1.3290000e-01 -7.4900000e-02 /
CHEB / 2.3338000e-01 3.9003000e-01 1.6846000e-01 -7.0205000e-04 /
CHEB / -9.6516000e-02 -6.3774000e-02 5.8308000e-02 2.3571000e-02 /

C4H7O_1_2+H(+m)=C4H7OJ(8)+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
4.4194283277852975 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.7659000e+00 -2.5228000e+00 -1.8340000e-01 1.4871000e-02 /
CHEB / 4.0563000e+00 1.9670000e+00 -7.1952000e-02 -3.2584000e-02 /
CHEB / 3.3086000e-01 6.4834000e-01 1.3061000e-01 -2.4406000e-02 /
CHEB / -1.8964000e-01 2.3058000e-02 9.3565000e-02 7.3041000e-03 /

C4H7-11+OH(+m)=C4H7OJ(8)+H(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -28.82302386808645
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.2467000e+00 -1.3343000e+00 -4.1427000e-01 2.0739000e-03 /
CHEB / 1.5567000e+00 1.2650000e+00 3.0051000e-01 -5.5713000e-02 /
CHEB / 1.6539000e-01 2.2969000e-01 1.4170000e-01 2.7172000e-02 /
CHEB / -5.4798000e-02 -7.1083000e-02 1.6008000e-02 2.7483000e-02 /

C4H7OJ(12)+H(+m)=C4H7OJ(8)+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
6.189612012381865 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.8975000e+00 -1.1986000e+00 -9.7662000e-02 9.7269000e-03 /
CHEB / 2.5555000e+00 1.0298000e+00 -1.6887000e-02 -2.0572000e-02 /
CHEB / 3.3591000e-01 2.9979000e-01 8.6401000e-02 -9.5294000e-03 /
CHEB / -6.3242000e-02 -3.1982000e-02 4.8479000e-02 1.1512000e-02 /

C4H7OJ(8)+H(+m)=CH3+C3H5OJ(13)(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) =
0.038472923887811206 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.5422000e+00 -1.2633000e+00 -8.1759000e-02 6.0967000e-03 /
CHEB / 2.9588000e+00 1.0317000e+00 -3.6792000e-02 -1.3854000e-02 /
CHEB / 2.1635000e-01 3.5190000e-01 7.4566000e-02 -1.2352000e-02 /
CHEB / -1.1693000e-01 -9.6272000e-03 5.6824000e-02 7.6301000e-03 /

C4H7OJ(16)+H(+m)=C4H7OJ(8)+H(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
12.098773974071534 kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.8102000e+00 -1.0367000e+00 -1.4554000e-01 1.9476000e-02 /
CHEB / 1.9119000e+00 9.6871000e-01 4.6550000e-02 -4.0000000e-02 /
CHEB / 3.0540000e-01 2.0558000e-01 1.0052000e-01 4.8661000e-04 /
CHEB / -1.5675000e-02 -6.0538000e-02 3.0344000e-02 1.8097000e-02 /

C4H7OJ(8)+H(+m)=C2H5+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -5.213256401191385
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0401000e+01 -1.3193000e+00 -7.1105000e-02 3.8900000e-03 /
CHEB / 2.0728000e+00 1.0085000e+00 -4.7279000e-02 -1.0038000e-02 /
CHEB / 1.5388000e-01 3.9880000e-01 5.8683000e-02 -1.2601000e-02 /
CHEB / -1.5073000e-01 2.5161000e-02 5.8982000e-02 3.7552000e-03 /

C4H7OJ(13)+H(+m)=C4H7OJ(8)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -
9.91921373770409 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.0202000e+00 -1.1054000e+00 -1.2483000e-01 1.5815000e-02 /
CHEB / 2.0367000e+00 1.0066000e+00 1.6835000e-02 -3.1952000e-02 /
CHEB / 3.2031000e-01 2.3944000e-01 9.8930000e-02 -4.9371000e-03 /
CHEB / -3.5580000e-02 -5.4255000e-02 3.8889000e-02 1.6187000e-02 /

C4H7OJ(8)+H(+m)=C3H7-1+HCO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -5.859394940357092
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0695000e+01 -1.3235000e+00 -7.0425000e-02 3.7640000e-03 /
CHEB / 2.1010000e+00 1.0059000e+00 -4.7904000e-02 -9.8158000e-03 /
CHEB / 1.6849000e-01 4.0221000e-01 5.7395000e-02 -1.2584000e-02 /
CHEB / -1.4688000e-01 2.8298000e-02 5.8971000e-02 3.4686000e-03 /

nC4H8O(+m)=C3H8+CO(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -1.8068306527267346
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.1643000e+01 3.1880000e-01 -3.9285000e-02 5.6099000e-04 /
CHEB / 2.5595000e+01 5.6536000e-01 -5.9611000e-02 -1.9138000e-03 /
CHEB / -4.9548000e-01 3.9472000e-01 -2.0567000e-02 -6.1673000e-03 /
CHEB / -3.5807000e-01 2.1463000e-01 9.4124000e-03 -6.0428000e-03 /

C4H8O-enol(+m)=C3H8+CO(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -8.996285903295945
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.1826000e+01 -1.2349000e+00 -1.0463000e-01 5.7398000e-03 /
CHEB / 2.5296000e+01 1.3024000e+00 -1.4698000e-01 -5.4818000e-04 /
CHEB / -1.3757000e-01 8.0595000e-01 -3.3597000e-02 -1.5135000e-02 /
CHEB / -4.0222000e-01 3.5448000e-01 3.2996000e-02 -1.3809000e-02 /
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CH3+C3H5O-enol2(+m)=C3H8+CO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -84.95292473096619
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 3.8763000e+00 -2.7640000e+00 -1.3915000e-01 6.2775000e-03 /
CHEB / 5.6035000e+00 1.8653000e+00 -1.1972000e-01 -1.6213000e-02 /
CHEB / 4.3720000e-01 7.9771000e-01 7.1628000e-02 -2.5659000e-02 /
CHEB / -2.2887000e-01 1.3186000e-01 9.2054000e-02 -3.6437000e-03 /

C4H7OJ(9)+H(+m)=C3H8+CO(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -113.0012924807186
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.1429000e+00 -1.8358000e+00 -3.6372000e-01 3.4568000e-02 /
CHEB / 1.9787000e+00 1.6428000e+00 1.7342000e-01 -7.9803000e-02 /
CHEB / 2.2187000e-01 3.7149000e-01 1.7000000e-01 1.0003000e-03 /
CHEB / -7.0041000e-02 -5.8443000e-02 5.4381000e-02 2.6062000e-02 /

C2H5+C2H3O-1(+m)=C3H8+CO(+m)        1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -109.07107085901127 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.8344000e+00 -1.9810000e+00 -3.3235000e-01 3.6471000e-02 /
CHEB / 2.2753000e+00 1.7396000e+00 1.2368000e-01 -7.6985000e-02 /
CHEB / 2.4252000e-01 4.1818000e-01 1.7000000e-01 -5.0997000e-03 /
CHEB / -9.1322000e-02 -5.0970000e-02 6.4913000e-02 2.2559000e-02 /

C4H7O_1_2+H(+m)=C3H8+CO(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -95.21317081809718
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.1013000e+00 -2.5898000e+00 -1.7259000e-01 1.3175000e-02 /
CHEB / 3.9505000e+00 1.9464000e+00 -8.7885000e-02 -2.8408000e-02 /
CHEB / 3.7501000e-01 6.9520000e-01 1.1609000e-01 -2.6333000e-02 /
CHEB / -1.8471000e-01 5.3207000e-02 9.6017000e-02 3.7451000e-03 /

C4H7-11+OH(+m)=C3H8+CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -119.61676635839834 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.2774000e+00 -1.3400000e+00 -4.2517000e-01 4.8634000e-03 /
CHEB / 1.6857000e+00 1.2595000e+00 3.0400000e-01 -6.1016000e-02 /
CHEB / 1.7680000e-01 2.4142000e-01 1.4756000e-01 2.6510000e-02 /
CHEB / -5.1270000e-02 -6.5152000e-02 1.9773000e-02 2.9253000e-02 /

C4H7OJ(12)+H(+m)=C3H8+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -96.98335450269374
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.2391000e+00 -1.2382000e+00 -9.1051000e-02 8.8190000e-03 /
CHEB / 2.4275000e+00 1.0204000e+00 -2.6603000e-02 -1.7939000e-02 /
CHEB / 3.4455000e-01 3.3359000e-01 7.8195000e-02 -1.1225000e-02 /
CHEB / -5.8500000e-02 -1.1355000e-02 5.2565000e-02 9.0018000e-03 /
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CH3+C3H5OJ(13)(+m)=C3H8+CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -90.8322154141997
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.5775000e+00 -1.3070000e+00 -7.3742000e-02 4.5053000e-03 /
CHEB / 2.9459000e+00 1.0136000e+00 -4.5117000e-02 -1.0943000e-02 /
CHEB / 3.7131000e-01 3.8882000e-01 6.2399000e-02 -1.2720000e-02 /
CHEB / -7.1925000e-02 1.7619000e-02 5.8797000e-02 4.5810000e-03 /

C4H7OJ(16)+H(+m)=C3H8+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -102.8925164643834
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.0373000e+00 -1.0662000e+00 -1.4358000e-01 2.0650000e-02 /
CHEB / 1.8869000e+00 9.6749000e-01 3.8523000e-02 -3.9783000e-02 /
CHEB / 2.9987000e-01 2.3127000e-01 9.8792000e-02 -2.4334000e-03 /
CHEB / -1.1995000e-02 -4.8586000e-02 3.5864000e-02 1.7111000e-02 /

C2H5+CH2CHO(+m)=C3H8+CO(+m)         1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -85.5804860891205 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.3609000e+00 -1.3661000e+00 -6.2506000e-02 2.0702000e-03 /
CHEB / 3.6854000e+00 9.8005000e-01 -5.3298000e-02 -7.4691000e-03 /
CHEB / 3.9375000e-01 4.3474000e-01 4.3793000e-02 -1.1721000e-02 /
CHEB / -1.1425000e-01 5.8858000e-02 5.7639000e-02 8.2777000e-04 /

C4H7OJ(13)+H(+m)=C3H8+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -100.71295622801597
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.2883000e+00 -1.1397000e+00 -1.2059000e-01 1.6034000e-02 /
CHEB / 1.9764000e+00 1.0037000e+00 7.2865000e-03 -3.0432000e-02 /
CHEB / 3.1770000e-01 2.6889000e-01 9.4806000e-02 -7.6385000e-03 /
CHEB / -3.1285000e-02 -3.9412000e-02 4.4375000e-02 1.4458000e-02 /

C3H7-1+HCO(+m)=C3H8+CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nC4H8O) deltaHrxn(T=298K) = -84.9343475499548 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.4068000e+00 -1.3707000e+00 -6.1795000e-02 1.9370000e-03 /
CHEB / 3.8661000e+00 9.7659000e-01 -5.3718000e-02 -7.2864000e-03 /
CHEB / 3.9423000e-01 4.3790000e-01 4.2337000e-02 -1.1614000e-02 /
CHEB / -1.1808000e-01 6.2480000e-02 5.7327000e-02 5.7240000e-04 /

C4H7OJ(8)+H(+m)=C3H8+CO(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (nC4H8O)  deltaHrxn(T=298K) = -90.79374249031189
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.8977000e+00 -1.3193000e+00 -7.1105000e-02 3.8900000e-03 /
CHEB / 3.0937000e+00 1.0085000e+00 -4.7279000e-02 -1.0038000e-02 /
CHEB / 3.7931000e-01 3.9880000e-01 5.8683000e-02 -1.2601000e-02 /
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CHEB / -8.4362000e-02 2.5161000e-02 5.8982000e-02 3.7552000e-03 /

!PDepNetwork C4H8O-enol2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-enol2       -37.68      83.04 23.93 29.26 34.16 38.51 45.56
      50.76 58.66 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H7O-13          -2.41 79.66 27.06 31.99 36.04 39.42 44.8  48.92
      55.62  !MRH CBS-QB3 w/1DHR corrections
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H7O_1_2         -8.11 80.56 25.48 30.4  34.84 38.6  44.45 48.8
      55.64  !MRH CBS-QB3 w/1DHR corrections
!Here are the path reactions and their high-P limit kinetics:
!     C4H7O-13+H=C4H8O-enol2  5.0000000e+13      0.00000
0.0000000e+00
!     pC3H5+CH2OH=C4H8O-enol2 1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7-24+OH=C4H8O-enol2  1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7O_1_2+H=C4H8O-enol2 5.0000000e+13      0.00000
0.0000000e+00

C4H7O-13+H(+m)=C4H8O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
87.36003224494898 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3148000e+01 3.8626000e-01 -3.9121000e-02 /
CHEB / -1.1074000e+00 7.0893000e-01 -6.3465000e-02 /
CHEB / -9.3845000e-01 5.4487000e-01 -2.8364000e-02 /
CHEB / -6.7341000e-01 3.4292000e-01 7.3223000e-03 /
CHEB / -4.6546000e-01 1.6566000e-01 2.7980000e-02 /

C4H7O-13+H(+m)=C4H7-24+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
6.218588643534961 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0061000e+01 -1.4767000e+00 -4.2625000e-02 /
CHEB / 2.7238000e+00 9.0116000e-01 -5.3724000e-02 /
CHEB / 3.9054000e-01 5.5697000e-01 1.0308000e-02 /
CHEB / -2.4816000e-01 2.0503000e-01 5.1913000e-02 /
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CHEB / -2.3557000e-01 -1.6523000e-02 4.8029000e-02 /

C4H7O-13+H(+m)=C4H7O_1_2+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
5.699201520767922 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6290000e+00 -1.4787000e+00 -4.2418000e-02 /
CHEB / 3.4602000e+00 8.9871000e-01 -5.3696000e-02 /
CHEB / 5.9465000e-01 5.5751000e-01 9.7604000e-03 /
CHEB / -1.7436000e-01 2.0738000e-01 5.1392000e-02 /
CHEB / -2.0816000e-01 -1.4445000e-02 4.8067000e-02 /

pC3H5+CH2OH(+m)=C4H8O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     C_rad/H2/O      deltaHrxn(T=298K) = -
99.33962250825837 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1723000e+01 6.3469000e-01 -9.5831000e-02 /
CHEB / -1.5775000e+00 1.1063000e+00 -1.3678000e-01 /
CHEB / -1.3086000e+00 7.5398000e-01 -4.1593000e-02 /
CHEB / -8.7544000e-01 3.9460000e-01 2.6789000e-02 /
CHEB / -5.4819000e-01 1.4393000e-01 4.5247000e-02 /

pC3H5+CH2OH(+m)=C4H7O-13+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
11.979590263309383 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6397000e+00 -1.3767000e+00 -5.9439000e-02 /
CHEB / 2.7681000e+00 9.9781000e-01 -5.1717000e-02 /
CHEB / 4.5723000e-01 4.9689000e-01 4.5480000e-02 /
CHEB / -1.2049000e-01 8.8765000e-02 7.2707000e-02 /
CHEB / -1.3665000e-01 -8.6778000e-02 3.5197000e-02 /

pC3H5+CH2OH(+m)=C4H7-24+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
18.19817890684435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0255000e+01 -1.3934000e+00 -5.8018000e-02 /
CHEB / 1.4329000e+00 9.8174000e-01 -5.3298000e-02 /
CHEB / 1.0669000e-01 5.0879000e-01 4.0085000e-02 /
CHEB / -2.2757000e-01 1.0960000e-01 7.1129000e-02 /
CHEB / -1.8395000e-01 -7.5538000e-02 3.9107000e-02 /

pC3H5+CH2OH(+m)=C4H7O_1_2+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
17.678791784077312 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7945000e+00 -1.3949000e+00 -5.7913000e-02 /
CHEB / 2.1989000e+00 9.8023000e-01 -5.3447000e-02 /
CHEB / 3.0700000e-01 5.0978000e-01 3.9612000e-02 /
CHEB / -1.5607000e-01 1.1151000e-01 7.0977000e-02 /
CHEB / -1.5618000e-01 -7.4418000e-02 3.9451000e-02 /
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C4H7-24+OH(+m)=C4H8O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     O_pri_rad      deltaHrxn(T=298K) = -
81.14144360141401 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2311000e+01 3.2329000e-01 -2.8294000e-02 /
CHEB / -1.1064000e+00 5.9931000e-01 -4.6700000e-02 /
CHEB / -8.5778000e-01 4.7464000e-01 -2.2305000e-02 /
CHEB / -6.4119000e-01 3.1474000e-01 4.4849000e-03 /
CHEB / -4.5495000e-01 1.6585000e-01 2.2604000e-02 /

C4H7O_1_2+H(+m)=C4H8O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeO     H_rad       deltaHrxn(T=298K) = -
81.66083072418107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3376000e+01 3.1772000e-01 -2.7410000e-02 /
CHEB / -1.0725000e+00 5.8950000e-01 -4.5299000e-02 /
CHEB / -8.1899000e-01 4.6810000e-01 -2.1739000e-02 /
CHEB / -6.1254000e-01 3.1185000e-01 4.3046000e-03 /
CHEB / -4.3756000e-01 1.6563000e-01 2.2149000e-02 /

C4H7O_1_2+H(+m)=C4H7-24+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #105 (C4H8O-enol2)      deltaHrxn(T=298K) = -
0.5193871227670392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3357000e+00 -1.5023000e+00 -3.9520000e-02 /
CHEB / 3.5090000e+00 8.6889000e-01 -5.2655000e-02 /
CHEB / 4.4223000e-01 5.6252000e-01 3.4042000e-03 /
CHEB / -2.7699000e-01 2.3429000e-01 4.4563000e-02 /
CHEB / -2.6211000e-01 1.0473000e-02 4.7463000e-02 /

!PDepNetwork C4H8O-enol3
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-enol3       -35.91      84.25 23.67 29.6  34.76 39.15 46.07
      51.14 56.94 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H7O-13          -2.41 79.66 27.06 31.99 36.04 39.42 44.8  48.92
      55.62  !MRH CBS-QB3 w/1DHR corrections
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
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!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H7O-14          7.38  85.17 24.32 29.59 34.01 37.72 43.55 47.83
      52.47 null
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C2H5O-1=C4H8O-enol3      1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+CH2OH=C4H8O-enol3 1.1500000e+13      0.00000
0.0000000e+00
!     C4H7O-13+H=C4H8O-enol3  5.0000000e+13      0.00000
0.0000000e+00
!     C4H7-14+OH=C4H8O-enol3  7.7000000e+13      0.00000
0.0000000e+00
!     C4H7O-14+H=C4H8O-enol3  5.0000000e+13      0.00000
0.0000000e+00
!     C4H6-13+H2O=C4H8O-enol3 2.2700000e+02      2.74000
5.6900000e+04
!     C2H4O+C2H4=C4H8O-enol3  1.6297242e+02      2.92024
4.4628571e+04

C2H3+C2H5O-1(+m)=C4H8O-enol3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     C_rad/H2/Cs           deltaHrxn(T=298K) = -
102.30922281094277 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9694000e+00 2.6144000e+00 -7.7566000e-01 /
CHEB / -3.0921000e+00 1.6914000e+00 8.4486000e-02 /
CHEB / -1.9665000e+00 6.8327000e-01 1.2856000e-01 /
CHEB / -1.1172000e+00 1.8410000e-01 7.1631000e-02 /
CHEB / -6.3038000e-01 1.4751000e-02 1.9574000e-02 /

C2H3+C2H5O-1(+m)=aC3H5+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
28.20697938051002 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2169000e+01 -7.2294000e-01 -2.2810000e-01 /
CHEB / 4.4527000e-01 7.2198000e-01 1.7866000e-01 /
CHEB / 2.9775000e-03 1.2833000e-01 9.0114000e-02 /
CHEB / -6.9143000e-02 -6.6251000e-02 -6.6758000e-04 /
CHEB / -5.6912000e-02 -5.9794000e-02 -2.8185000e-02 /

C2H3+C2H5O-1(+m)=C4H7O-13+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
16.719027692158342 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3337000e+00 -7.2597000e-01 -2.1519000e-01 /
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CHEB / 2.0095000e+00 7.4775000e-01 1.7220000e-01 /
CHEB / 4.7640000e-01 1.0776000e-01 8.5339000e-02 /
CHEB / 8.3945000e-02 -7.8369000e-02 -6.0937000e-03 /
CHEB / -2.3537000e-03 -5.7299000e-02 -2.8966000e-02 /

C2H3+C2H5O-1(+m)=C4H7-14+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
8.829031560988266 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7178000e+00 -7.0994000e-01 -2.0538000e-01 /
CHEB / 1.8289000e+00 7.5909000e-01 1.7009000e-01 /
CHEB / 4.3410000e-01 7.5949000e-02 7.9949000e-02 /
CHEB / 4.1931000e-02 -8.6810000e-02 -1.2850000e-02 /
CHEB / -2.3217000e-02 -5.0286000e-02 -2.9037000e-02 /

C2H3+C2H5O-1(+m)=C4H7O-14+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
6.929671028403909 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7488000e+00 -7.0581000e-01 -2.0428000e-01 /
CHEB / 2.4707000e+00 7.5881000e-01 1.7020000e-01 /
CHEB / 5.9645000e-01 7.0739000e-02 7.9054000e-02 /
CHEB / 9.4422000e-02 -8.7326000e-02 -1.3899000e-02 /
CHEB / -2.7391000e-03 -4.8986000e-02 -2.8918000e-02 /

C2H3+C2H5O-1(+m)=C4H6-13+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
95.91015972579794 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6771000e+00 -7.0660000e-01 -2.4114000e-01 /
CHEB / 1.3787000e+00 6.9478000e-01 1.8755000e-01 /
CHEB / 1.7536000e-01 1.3587000e-01 9.4306000e-02 /
CHEB / -1.0446000e-02 -5.7628000e-02 2.6238000e-03 /
CHEB / -3.1395000e-02 -5.9553000e-02 -2.7842000e-02 /

C2H3+C2H5O-1(+m)=C2H4O+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
81.97139864035303 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5839000e+00 -7.1069000e-01 -2.3851000e-01 /
CHEB / 1.2303000e+00 7.0016000e-01 1.8559000e-01 /
CHEB / 1.5086000e-01 1.3511000e-01 9.3471000e-02 /
CHEB / -1.7968000e-02 -5.9004000e-02 2.0945000e-03 /
CHEB / -3.4572000e-02 -5.9666000e-02 -2.7850000e-02 /

aC3H5+CH2OH(+m)=C4H8O-enol3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_rad/H2/O           deltaHrxn(T=298K) = -
74.10224343043274 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2472000e+01 4.4433000e-01 -3.5443000e-02 /
CHEB / -1.6497000e+00 7.9236000e-01 -5.0851000e-02 /
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CHEB / -1.2219000e+00 5.5689000e-01 -8.1551000e-03 /
CHEB / -8.6738000e-01 2.9607000e-01 2.5007000e-02 /
CHEB / -5.6898000e-01 1.0117000e-01 3.2386000e-02 /

aC3H5+CH2OH(+m)=C4H6-13+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
67.70318034528792 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9110000e+00 -1.4166000e+00 -4.3225000e-02 /
CHEB / 2.8390000e+00 9.6816000e-01 -4.6092000e-02 /
CHEB / 4.3207000e-01 5.2676000e-01 2.6133000e-02 /
CHEB / -1.5716000e-01 1.3002000e-01 5.6590000e-02 /
CHEB / -1.5558000e-01 -6.7364000e-02 3.4930000e-02 /

aC3H5+CH2OH(+m)=C2H4O+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
53.76441925984302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6530000e+00 -1.4066000e+00 -4.4424000e-02 /
CHEB / 2.8199000e+00 9.7861000e-01 -4.6094000e-02 /
CHEB / 4.1115000e-01 5.2074000e-01 2.9012000e-02 /
CHEB / -1.6866000e-01 1.1752000e-01 5.8355000e-02 /
CHEB / -1.5512000e-01 -7.4971000e-02 3.3717000e-02 /

C4H7O-13+H(+m)=C4H8O-enol3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
85.59019511878442 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2566000e+01 7.4041000e-01 -1.0639000e-01 /
CHEB / -1.9912000e+00 1.1947000e+00 -1.1118000e-01 /
CHEB / -1.5129000e+00 6.9452000e-01 7.1948000e-03 /
CHEB / -9.6507000e-01 2.8455000e-01 5.2023000e-02 /
CHEB / -5.8785000e-01 6.2262000e-02 3.8386000e-02 /

C4H7O-13+H(+m)=aC3H5+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
11.487951688351677 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2152000e+01 -1.2461000e+00 -8.1412000e-02 /
CHEB / 1.5715000e+00 1.0633000e+00 -2.8537000e-02 /
CHEB / 1.5783000e-01 3.7291000e-01 8.4679000e-02 /
CHEB / -1.2654000e-01 -2.7163000e-02 6.5032000e-02 /
CHEB / -9.6071000e-02 -1.1088000e-01 2.4977000e-03 /

C4H7O-13+H(+m)=C4H6-13+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
79.19113203363959 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1409000e+00 -1.2913000e+00 -7.5867000e-02 /
CHEB / 2.1497000e+00 1.0384000e+00 -3.5982000e-02 /
CHEB / 2.8925000e-01 4.1884000e-01 7.2507000e-02 /
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CHEB / -6.5405000e-02 1.6463000e-02 6.8759000e-02 /
CHEB / -7.6256000e-02 -1.0222000e-01 1.4067000e-02 /

C4H7O-13+H(+m)=C2H4O+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
65.25237094819468 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9654000e+00 -1.2840000e+00 -7.6547000e-02 /
CHEB / 2.0555000e+00 1.0433000e+00 -3.4805000e-02 /
CHEB / 2.7410000e-01 4.1169000e-01 7.4463000e-02 /
CHEB / -7.2325000e-02 8.5897000e-03 6.8270000e-02 /
CHEB / -7.8288000e-02 -1.0451000e-01 1.2102000e-02 /

C4H7-14+OH(+m)=C4H8O-enol3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     O_pri_rad           deltaHrxn(T=298K) = -
93.48019124995449 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2266000e+01 1.3154000e+00 -3.1240000e-01 /
CHEB / -2.5886000e+00 1.5607000e+00 -1.1170000e-01 /
CHEB / -1.7518000e+00 7.3455000e-01 5.7851000e-02 /
CHEB / -1.0629000e+00 2.4027000e-01 7.0267000e-02 /
CHEB / -6.2133000e-01 3.5228000e-02 3.0988000e-02 /

C4H7-14+OH(+m)=aC3H5+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
19.37794781952175 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3010000e+01 -1.0453000e+00 -1.5291000e-01 /
CHEB / 8.4270000e-01 9.8031000e-01 5.4114000e-02 /
CHEB / 7.7810000e-02 2.3981000e-01 1.1167000e-01 /
CHEB / -1.0191000e-01 -6.5649000e-02 3.7452000e-02 /
CHEB / -8.3342000e-02 -8.9323000e-02 -2.0363000e-02 /

C4H7-14+OH(+m)=C4H7O-13+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
7.889996131170072 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8552000e+00 -1.0018000e+00 -1.5200000e-01 /
CHEB / 2.6806000e+00 9.8746000e-01 6.3275000e-02 /
CHEB / 5.6784000e-01 1.8984000e-01 1.1272000e-01 /
CHEB / 4.2665000e-02 -8.8893000e-02 2.5009000e-02 /
CHEB / -2.8053000e-02 -8.3238000e-02 -2.7283000e-02 /

C4H7-14+OH(+m)=C4H6-13+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
87.08112816480967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7321000e+00 -1.0641000e+00 -1.5866000e-01 /
CHEB / 1.6311000e+00 9.6652000e-01 5.1322000e-02 /
CHEB / 2.2210000e-01 2.6605000e-01 1.1273000e-01 /
CHEB / -4.4134000e-02 -4.5948000e-02 4.5517000e-02 /
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CHEB / -5.8877000e-02 -8.8472000e-02 -1.4921000e-02 /

C4H7-14+OH(+m)=C2H4O+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
73.14236707936476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0601000e+01 -1.0616000e+00 -1.5734000e-01 /
CHEB / 1.5059000e+00 9.6917000e-01 5.1665000e-02 /
CHEB / 2.0308000e-01 2.6205000e-01 1.1236000e-01 /
CHEB / -5.1042000e-02 -4.9353000e-02 4.4072000e-02 /
CHEB / -6.1740000e-02 -8.8848000e-02 -1.5895000e-02 /

C4H7O-14+H(+m)=C4H8O-enol3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/CsO     H_rad          deltaHrxn(T=298K) = -
95.37955178253884 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2094000e+01 1.4281000e+00 -3.5596000e-01 /
CHEB / -2.6851000e+00 1.5947000e+00 -9.9679000e-02 /
CHEB / -1.7437000e+00 7.3346000e-01 6.5834000e-02 /
CHEB / -1.0291000e+00 2.3383000e-01 7.1350000e-02 /
CHEB / -5.8888000e-01 3.2405000e-02 2.9656000e-02 /

C4H7O-14+H(+m)=aC3H5+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
21.277308352106104 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2992000e+01 -1.0104000e+00 -1.6470000e-01 /
CHEB / 7.5177000e-01 9.5628000e-01 7.0505000e-02 /
CHEB / 1.0438000e-01 2.2411000e-01 1.1173000e-01 /
CHEB / -5.6000000e-02 -6.7289000e-02 3.2560000e-02 /
CHEB / -4.6124000e-02 -8.5766000e-02 -2.2337000e-02 /

C4H7O-14+H(+m)=C4H7O-13+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
9.789356663754425 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8815000e+00 -9.7337000e-01 -1.6098000e-01 /
CHEB / 2.5483000e+00 9.6559000e-01 7.6822000e-02 /
CHEB / 5.9448000e-01 1.7848000e-01 1.1125000e-01 /
CHEB / 8.9908000e-02 -8.8737000e-02 2.0950000e-02 /
CHEB / 8.8481000e-03 -8.0173000e-02 -2.8170000e-02 /

C4H7O-14+H(+m)=C4H7-14+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
1.8993605325843497 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9026000e+00 -8.9784000e-01 -1.7023000e-01 /
CHEB / 2.7541000e+00 9.3419000e-01 1.0046000e-01 /
CHEB / 5.1031000e-01 1.2033000e-01 1.0760000e-01 /
CHEB / 3.9276000e-02 -9.7841000e-02 5.1902000e-03 /
CHEB / -9.2237000e-03 -6.6941000e-02 -3.1734000e-02 /
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C4H7O-14+H(+m)=C4H6-13+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
88.98048869739402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6851000e+00 -1.0245000e+00 -1.7241000e-01 /
CHEB / 1.5606000e+00 9.4140000e-01 6.9742000e-02 /
CHEB / 2.5188000e-01 2.4750000e-01 1.1396000e-01 /
CHEB / 1.6929000e-03 -4.9506000e-02 4.0223000e-02 /
CHEB / -2.1510000e-02 -8.5116000e-02 -1.7787000e-02 /

C4H7O-14+H(+m)=C2H4O+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
75.04172761194911 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0559000e+01 -1.0228000e+00 -1.7072000e-01 /
CHEB / 1.4322000e+00 9.4426000e-01 6.9693000e-02 /
CHEB / 2.3218000e-01 2.4401000e-01 1.1337000e-01 /
CHEB / -5.2704000e-03 -5.2549000e-02 3.8849000e-02 /
CHEB / -2.4411000e-02 -8.5427000e-02 -1.8593000e-02 /

C4H6-13+H2O(+m)=C4H8O-enol3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: 1,3_Insertion_ROR estimate:
(Average:) Cd/H/De_Cd/H2     H_OH         deltaHrxn(T=298K) = -
6.399063085144828 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3785000e+01 2.9498000e-01 -1.3688000e-02 /
CHEB / 1.9346000e+01 5.4218000e-01 -2.0340000e-02 /
CHEB / -6.2950000e-01 4.1730000e-01 -3.6088000e-03 /
CHEB / -6.0880000e-01 2.6042000e-01 1.3054000e-02 /
CHEB / -4.6603000e-01 1.1963000e-01 2.1587000e-02 /

C2H4O+C2H4(+m)=C4H8O-enol3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3) High-P Limit: 1,3_Insertion_ROR estimate:
(Average:) Cd_pri_OH     Cd/unsub_Cd/unsub      deltaHrxn(T=298K) = -
20.337824170589727 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.4585000e+00 3.1877000e-01 -1.6543000e-02 /
CHEB / 1.5229000e+01 5.8330000e-01 -2.4582000e-02 /
CHEB / -6.6607000e-01 4.4282000e-01 -4.6490000e-03 /
CHEB / -6.4397000e-01 2.6949000e-01 1.4509000e-02 /
CHEB / -4.8737000e-01 1.1813000e-01 2.3377000e-02 /

C2H4O+C2H4(+m)=C4H6-13+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #155 (C4H8O-enol3)      deltaHrxn(T=298K) = -
13.938761085444902 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4177000e+01 -1.4750000e+00 -3.4193000e-02 /
CHEB / 2.0489000e+01 9.0248000e-01 -4.2427000e-02 /
CHEB / 8.9679000e-01 5.5362000e-01 1.0058000e-02 /
CHEB / -9.0366000e-02 1.9959000e-01 4.2747000e-02 /
CHEB / -1.6686000e-01 -1.8341000e-02 3.7230000e-02 /
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!PDepNetwork MEK
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     MEK               -56.88      81.06 24.17 29.7  34.59 38.84 46.03
      51.35 58.84 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H5OJ(8)         -6.18 74.68 17.76 20.93 24.04 26.82 31.36 34.8
      40.18
!     cH2C[O]C2H5       -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH2C[O]CH3        -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17
      41.25
!     CH3C[O]cHCH3            -10.78      80.09 23.09 27.78 31.99 35.82
      42.42 47.34 54.59 null
!     CH3C[O]CH2cH2           -7.88 84.48 23.4  28.34 32.68 36.44 42.87
      47.61 54.18 null
!     C3H8              -24.27      66.07 17.76 22.39 26.7  30.47 36.6
      41.32 48.85
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H5OJ(8)=MEK             4.0400000e+15      -0.80000
0.0000000e+00
!     cH2C[O]C2H5+H=MEK             5.0000000e+13      0.00000
0.0000000e+00
!     CH3CO+C2H5=MEK          3.1200000e+14      -0.50000
0.0000000e+00
!     CH2C[O]CH3+CH3=MEK            2.4874006e+15      -0.90000
2.5000000e+02
!     CH3C[O]cHCH3+H=MEK            5.0000000e+13      0.00000
0.0000000e+00
!     CH3C[O]CH2cH2+H=MEK           1.0000000e+14      0.00000
0.0000000e+00
!     C3H8+CO=MEK             5.3800000e+02      3.29000
1.0450000e+05

CH3+C3H5OJ(8)(+m)=MEK(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK) High-P Limit: R_Recombination exact:  C_methyl
CO_rad/NonDe      deltaHrxn(T=298K) = -85.94091634334336 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2806000e+01 4.4079000e-01 -3.7398000e-02 /
CHEB / -1.8586000e+00 7.5855000e-01 -4.4889000e-02 /
CHEB / -1.1488000e+00 4.8961000e-01 5.4289000e-03 /
CHEB / -7.1696000e-01 2.3143000e-01 3.2056000e-02 /
CHEB / -4.3309000e-01 6.8472000e-02 2.8726000e-02 /
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CH3+C3H5OJ(8)(+m)=CH3CO+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -1.5893939700067854 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1278000e+01 -1.2656000e+00 -6.7802000e-02 /
CHEB / 1.5579000e+00 1.0516000e+00 -2.8736000e-02 /
CHEB / 6.6124000e-02 3.7657000e-01 6.8739000e-02 /
CHEB / -1.9893000e-01 -9.8517000e-03 5.2560000e-02 /
CHEB / -1.0601000e-01 -9.3754000e-02 4.2922000e-03 /

CH3+C3H5OJ(8)(+m)=C3H8+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -79.77158699210835 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4186000e-01 -3.9317000e-01 -1.9728000e-01 /
CHEB / 1.0032000e+01 3.7349000e-01 1.8093000e-01 /
CHEB / 4.5412000e-01 9.7529000e-02 5.0962000e-02 /
CHEB / 1.3706000e-01 -4.2317000e-02 -1.3493000e-02 /
CHEB / 4.1638000e-02 -3.5908000e-02 -1.7519000e-02 /

cH2C[O]C2H5+H(+m)=MEK(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK) High-P Limit: R_Recombination estimate: (Average:)
C_rad/H2/CO     H_rad         deltaHrxn(T=298K) = -101.08918543693605
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2429000e+01 1.2707000e+00 -3.3995000e-01 /
CHEB / -2.0159000e+00 9.1786000e-01 1.0200000e-01 /
CHEB / -1.3245000e+00 5.2941000e-01 5.0389000e-02 /
CHEB / -7.6343000e-01 1.6845000e-01 4.7285000e-02 /
CHEB / -4.2295000e-01 2.5176000e-02 2.2661000e-02 /

cH2C[O]C2H5+H(+m)=CH3+C3H5OJ(8)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -15.148269093592678 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2811000e+01 -8.6319000e-01 -1.9180000e-01 /
CHEB / 5.8679000e-01 8.1670000e-01 1.3227000e-01 /
CHEB / 1.6045000e-01 1.9172000e-01 8.0389000e-02 /
CHEB / -3.4980000e-02 -6.6526000e-02 1.5079000e-02 /
CHEB / -3.1593000e-02 -6.7523000e-02 -1.8569000e-02 /

cH2C[O]C2H5+H(+m)=CH3CO+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -16.73766306359946 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3025000e+01 -8.6818000e-01 -1.9271000e-01 /
CHEB / 4.2021000e-01 8.1542000e-01 1.3205000e-01 /
CHEB / 1.1267000e-01 1.9804000e-01 8.0517000e-02 /
CHEB / -4.9136000e-02 -6.4130000e-02 1.6219000e-02 /
CHEB / -3.7015000e-02 -6.8377000e-02 -1.8012000e-02 /

cH2C[O]C2H5+H(+m)=CH2C[O]CH3+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -15.118246338214405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / 1.1829000e+01 -8.6319000e-01 -1.9180000e-01 /
CHEB / 8.4147000e-01 8.1670000e-01 1.3227000e-01 /
CHEB / 2.2738000e-01 1.9172000e-01 8.0389000e-02 /
CHEB / -1.1532000e-02 -6.6526000e-02 1.5079000e-02 /
CHEB / -2.2363000e-02 -6.7523000e-02 -1.8569000e-02 /

cH2C[O]C2H5+H(+m)=CH3C[O]cHCH3+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -2.899671195239648
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5751000e+00 -7.6528000e-01 -1.8767000e-01 /
CHEB / 2.8428000e+00 7.8987000e-01 1.4440000e-01 /
CHEB / 6.8839000e-01 1.0220000e-01 7.6204000e-02 /
CHEB / 1.1137000e-01 -7.8521000e-02 -1.9658000e-03 /
CHEB / 3.0073000e-02 -5.0372000e-02 -2.2674000e-02 /

cH2C[O]C2H5+H(+m)=C3H8+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -94.91985608570103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2656000e+00 -3.8847000e-01 -1.8121000e-01 /
CHEB / 6.6265000e+00 4.0487000e-01 1.7911000e-01 /
CHEB / 9.0075000e-01 5.7758000e-02 3.5162000e-02 /
CHEB / 2.5683000e-01 -5.3880000e-02 -1.8487000e-02 /
CHEB / 8.4326000e-02 -2.7010000e-02 -1.5022000e-02 /

CH3CO+C2H5(+m)=MEK(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (MEK) High-P Limit: R_Recombination exact:  CO_rad/NonDe
C_rad/H2/Cs       deltaHrxn(T=298K) = -84.35152237333658 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2385000e+01 4.1920000e-01 -3.3093000e-02 /
CHEB / -1.5487000e+00 7.2873000e-01 -4.1323000e-02 /
CHEB / -1.0951000e+00 4.8046000e-01 3.7043000e-03 /
CHEB / -7.1515000e-01 2.3381000e-01 2.9755000e-02 /
CHEB / -4.3680000e-01 7.2321000e-02 2.8256000e-02 /

CH3CO+C2H5(+m)=C3H8+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -78.18219302210156 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2763000e+00 -3.9216000e-01 -1.9818000e-01 /
CHEB / 1.0608000e+01 3.7044000e-01 1.8093000e-01 /
CHEB / 4.6059000e-01 9.9314000e-02 5.1884000e-02 /
CHEB / 1.2272000e-01 -4.1259000e-02 -1.3108000e-02 /
CHEB / 3.4025000e-02 -3.6165000e-02 -1.7610000e-02 /

CH2C[O]CH3+CH3(+m)=MEK(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK) High-P Limit: R_Recombination estimate: (Average:)
C_rad/H2/CO     C_methyl      deltaHrxn(T=298K) = -85.97093909872164
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2133000e+01 4.4079000e-01 -3.7398000e-02 /
CHEB / -1.7529000e+00 7.5855000e-01 -4.4889000e-02 /
CHEB / -1.1560000e+00 4.8961000e-01 5.4289000e-03 /
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CHEB / -7.2011000e-01 2.3143000e-01 3.2056000e-02 /
CHEB / -4.3111000e-01 6.8472000e-02 2.8726000e-02 /

CH2C[O]CH3+CH3(+m)=CH3+C3H5OJ(8)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -0.030022755378277033
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0312000e+01 -1.2532000e+00 -7.0738000e-02 /
CHEB / 1.9161000e+00 1.0542000e+00 -2.6333000e-02 /
CHEB / 9.0650000e-02 3.6474000e-01 7.1963000e-02 /
CHEB / -1.8733000e-01 -1.6854000e-02 5.1684000e-02 /
CHEB / -9.6109000e-02 -9.3897000e-02 2.4960000e-03 /

CH2C[O]CH3+CH3(+m)=CH3CO+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -1.6194167253850615 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0605000e+01 -1.2656000e+00 -6.7802000e-02 /
CHEB / 1.6637000e+00 1.0516000e+00 -2.8736000e-02 /
CHEB / 5.8947000e-02 3.7657000e-01 6.8739000e-02 /
CHEB / -2.0208000e-01 -9.8517000e-03 5.2560000e-02 /
CHEB / -1.0403000e-01 -9.3754000e-02 4.2922000e-03 /

CH2C[O]CH3+CH3(+m)=C3H8+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -79.80160974748662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2147000e+00 -3.9317000e-01 -1.9728000e-01 /
CHEB / 1.0138000e+01 3.7349000e-01 1.8093000e-01 /
CHEB / 4.4695000e-01 9.7529000e-02 5.0962000e-02 /
CHEB / 1.3391000e-01 -4.2317000e-02 -1.3493000e-02 /
CHEB / 4.3620000e-02 -3.5908000e-02 -1.7519000e-02 /

CH3C[O]cHCH3+H(+m)=MEK(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK) High-P Limit: R_Recombination estimate: (Average:)
C_rad/H/OneDeC     H_rad      deltaHrxn(T=298K) = -98.1895142416964
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2617000e+01 9.6844000e-01 -2.1992000e-01 /
CHEB / -1.9336000e+00 9.8214000e-01 1.7476000e-02 /
CHEB / -1.2843000e+00 5.3168000e-01 4.1216000e-02 /
CHEB / -7.6340000e-01 1.8021000e-01 4.9426000e-02 /
CHEB / -4.3291000e-01 3.1862000e-02 2.4947000e-02 /

CH3C[O]cHCH3+H(+m)=CH3+C3H5OJ(8)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -12.24859789835303
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2576000e+01 -9.8164000e-01 -1.5806000e-01 /
CHEB / 7.9985000e-01 9.2024000e-01 8.2615000e-02 /
CHEB / 1.7127000e-01 2.1951000e-01 8.7384000e-02 /
CHEB / -6.4413000e-02 -6.5867000e-02 2.5631000e-02 /
CHEB / -5.0333000e-02 -7.5167000e-02 -1.6353000e-02 /
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CH3C[O]cHCH3+H(+m)=CH3CO+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -13.837991868359811 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2801000e+01 -9.8910000e-01 -1.5785000e-01 /
CHEB / 6.2225000e-01 9.2002000e-01 8.1333000e-02 /
CHEB / 1.2367000e-01 2.2720000e-01 8.6926000e-02 /
CHEB / -7.8175000e-02 -6.2957000e-02 2.7027000e-02 /
CHEB / -5.5988000e-02 -7.6097000e-02 -1.5496000e-02 /

CH3C[O]cHCH3+H(+m)=CH2C[O]CH3+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -12.218575142974757
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1593000e+01 -9.8164000e-01 -1.5806000e-01 /
CHEB / 1.0545000e+00 9.2024000e-01 8.2615000e-02 /
CHEB / 2.3820000e-01 2.1951000e-01 8.7384000e-02 /
CHEB / -4.0964000e-02 -6.5867000e-02 2.5631000e-02 /
CHEB / -4.1103000e-02 -7.5167000e-02 -1.6353000e-02 /

CH3C[O]cHCH3+H(+m)=C3H8+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -92.02018489046138 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5991000e+00 -3.9306000e-01 -1.8521000e-01 /
CHEB / 7.3289000e+00 4.0124000e-01 1.8002000e-01 /
CHEB / 8.2198000e-01 6.8282000e-02 3.8890000e-02 /
CHEB / 2.3052000e-01 -5.2613000e-02 -1.7641000e-02 /
CHEB / 7.0364000e-02 -2.9707000e-02 -1.5762000e-02 /

CH3C[O]CH2cH2+H(+m)=MEK(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK) High-P Limit: R_Recombination exact:  C_rad/H2/Cs
H_rad       deltaHrxn(T=298K) = -101.08918543693605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2730000e+01 1.2707000e+00 -3.3995000e-01 /
CHEB / -2.0159000e+00 9.1786000e-01 1.0200000e-01 /
CHEB / -1.3245000e+00 5.2941000e-01 5.0389000e-02 /
CHEB / -7.6343000e-01 1.6845000e-01 4.7285000e-02 /
CHEB / -4.2295000e-01 2.5176000e-02 2.2661000e-02 /

CH3C[O]CH2cH2+H(+m)=CH3+C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -15.148269093592678
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3112000e+01 -8.6319000e-01 -1.9180000e-01 /
CHEB / 5.8679000e-01 8.1670000e-01 1.3227000e-01 /
CHEB / 1.6045000e-01 1.9172000e-01 8.0389000e-02 /
CHEB / -3.4980000e-02 -6.6526000e-02 1.5079000e-02 /
CHEB / -3.1593000e-02 -6.7523000e-02 -1.8569000e-02 /

CH3C[O]CH2cH2+H(+m)=cH2C[O]C2H5+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 8.1551000e+00 -7.1920000e-01 -1.8906000e-01 /
CHEB / 3.3723000e+00 7.5740000e-01 1.5199000e-01 /
CHEB / 7.5258000e-01 7.7498000e-02 7.2948000e-02 /
CHEB / 1.2876000e-01 -7.4008000e-02 -7.7915000e-03 /
CHEB / 3.9837000e-02 -4.5616000e-02 -2.2110000e-02 /

CH3C[O]CH2cH2+H(+m)=CH3CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -16.73766306359946 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3326000e+01 -8.6818000e-01 -1.9271000e-01 /
CHEB / 4.2021000e-01 8.1542000e-01 1.3205000e-01 /
CHEB / 1.1267000e-01 1.9804000e-01 8.0517000e-02 /
CHEB / -4.9136000e-02 -6.4130000e-02 1.6219000e-02 /
CHEB / -3.7015000e-02 -6.8377000e-02 -1.8012000e-02 /

CH3C[O]CH2cH2+H(+m)=CH2C[O]CH3+CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -15.118246338214405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2130000e+01 -8.6319000e-01 -1.9180000e-01 /
CHEB / 8.4147000e-01 8.1670000e-01 1.3227000e-01 /
CHEB / 2.2738000e-01 1.9172000e-01 8.0389000e-02 /
CHEB / -1.1532000e-02 -6.6526000e-02 1.5079000e-02 /
CHEB / -2.2363000e-02 -6.7523000e-02 -1.8569000e-02 /

CH3C[O]CH2cH2+H(+m)=CH3C[O]cHCH3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (MEK)     deltaHrxn(T=298K) = -2.899671195239648
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8761000e+00 -7.6528000e-01 -1.8767000e-01 /
CHEB / 2.8428000e+00 7.8987000e-01 1.4440000e-01 /
CHEB / 6.8839000e-01 1.0220000e-01 7.6204000e-02 /
CHEB / 1.1137000e-01 -7.8521000e-02 -1.9658000e-03 /
CHEB / 3.0073000e-02 -5.0372000e-02 -2.2674000e-02 /

CH3C[O]CH2cH2+H(+m)=C3H8+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (MEK)    deltaHrxn(T=298K) = -94.91985608570103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5667000e+00 -3.8847000e-01 -1.8121000e-01 /
CHEB / 6.6265000e+00 4.0487000e-01 1.7911000e-01 /
CHEB / 9.0075000e-01 5.7758000e-02 3.5162000e-02 /
CHEB / 2.5683000e-01 -5.3880000e-02 -1.8487000e-02 /
CHEB / 8.4326000e-02 -2.7010000e-02 -1.5022000e-02 /

C3H8+CO(+m)=MEK(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (MEK) High-P Limit: 1,2_Insertion estimate: (Average:) C_methyl_C_pri
CO_birad          deltaHrxn(T=298K) = -6.169329351235014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4172000e+01 3.2284000e+00 -8.3900000e-01 /
CHEB / 3.5160000e+01 3.2279000e-01 3.2467000e-01 /
CHEB / -1.0572000e+00 3.7307000e-01 1.4610000e-01 /
CHEB / -6.8393000e-01 1.1983000e-01 4.5103000e-02 /
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CHEB / -3.8781000e-01 1.1947000e-02 1.2604000e-02 /

!PDepNetwork MEKenol
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     MEKenol           -46.68      81.2  24.43 29.77 34.47 38.61 45.55
      50.67 58.38 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CH3CHcOH          21.62 72.89 19.21 23.08 26.31 28.95 32.97 35.9
      40.57 null
!     CH2C[OH]cHCH3           -10.58      79.45 23.81 29.21 33.69 37.49
      43.71 48.21 54.89 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3C[OH]cH        20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23
      39.84 null
!     CH3C[OH]cCH3            10.22 83.01 24.09 28.56 32.53 36.09 42.21
      46.76 53.62 null
!     CH3C[OH]CHcH2           -10.58      79.45 23.81 29.21 33.69 37.49
      43.71 48.21 54.89 null
!     CH3C[O]cHCH3            -10.78      80.09 23.09 27.78 31.99 35.82
      42.42 47.34 54.59 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+CH3CHcOH=MEKenol    1.4157154e+13      -0.15000
2.9166667e+02
!     CH2C[OH]cHCH3+H=MEKenol       5.0000000e+13      0.00000
0.0000000e+00
!     C4H7-22+OH=MEKenol      1.4157154e+13      -0.15000
2.9166667e+02
!     CH3C[OH]cH+CH3=MEKenol        7.2300000e+13      0.00000
0.0000000e+00
!     CH3C[OH]cCH3+H=MEKenol        1.4157154e+13      -0.15000
2.9166667e+02
!     CH3C[OH]CHcH2+H=MEKenol       5.0000000e+13      0.00000
0.0000000e+00
!     CH3C[O]cHCH3+H=MEKenol        1.4157154e+13      -0.15000
2.9166667e+02

CH3+CH3CHcOH(+m)=MEKenol(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) C_methyl     Cd_rad/NonDe      deltaHrxn(T=298K) = -
103.53900990499244 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1928000e+01 4.9035000e-01 -6.2376000e-02 /
CHEB / -1.3433000e+00 8.7563000e-01 -9.7125000e-02 /
CHEB / -1.1139000e+00 6.2290000e-01 -3.8759000e-02 /
CHEB / -7.4694000e-01 3.4592000e-01 9.5027000e-03 /
CHEB / -4.7278000e-01 1.3901000e-01 2.7141000e-02 /
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```
CH3+CH3CHcOH(+m)=CH2C[OH]cHCH3+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -15.348512118907216
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3848000e+00 -1.4207000e+00 -4.4959000e-02 /
CHEB / 2.1055000e+00 9.6206000e-01 -4.8383000e-02 /
CHEB / 2.8332000e-01 5.2663000e-01 2.5349000e-02 /
CHEB / -1.5974000e-01 1.3373000e-01 5.7517000e-02 /
CHEB / -1.4994000e-01 -6.3636000e-02 3.7027000e-02 /

CH3+CH3CHcOH(+m)=CH3C[OH]cH+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -1.3298809274761751
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7713000e+00 -1.3503000e+00 -5.3265000e-02 /
CHEB / 2.9323000e+00 1.0284000e+00 -4.5325000e-02 /
CHEB / 3.3026000e-01 4.7451000e-01 4.7502000e-02 /
CHEB / -1.7031000e-01 4.8002000e-02 6.6268000e-02 /
CHEB / -1.1836000e-01 -1.0541000e-01 2.4114000e-02 /

CH3+CH3CHcOH(+m)=CH3C[OH]CHcH2+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -15.348512118907216
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3848000e+00 -1.4207000e+00 -4.4959000e-02 /
CHEB / 2.1055000e+00 9.6206000e-01 -4.8383000e-02 /
CHEB / 2.8332000e-01 5.2663000e-01 2.5349000e-02 /
CHEB / -1.5974000e-01 1.3373000e-01 5.7517000e-02 /
CHEB / -1.4994000e-01 -6.3636000e-02 3.7027000e-02 /

CH3+CH3CHcOH(+m)=CH3C[O]cHCH3+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -15.54844170184466
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4752000e+00 -1.4184000e+00 -4.5135000e-02 /
CHEB / 1.8033000e+00 9.6461000e-01 -4.8277000e-02 /
CHEB / 2.0386000e-01 5.2541000e-01 2.5984000e-02 /
CHEB / -1.8903000e-01 1.3082000e-01 5.7865000e-02 /
CHEB / -1.6057000e-01 -6.5583000e-02 3.6699000e-02 /

CH2C[OH]cHCH3+H(+m)=MEKenol(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
88.19049778608522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3374000e+01 2.7293000e-01 -2.3683000e-02 /
CHEB / -9.2526000e-01 5.0839000e-01 -4.0314000e-02 /
CHEB / -7.2828000e-01 4.0872000e-01 -2.2647000e-02 /
CHEB / -5.5365000e-01 2.7884000e-01 -2.5502000e-03 /
CHEB / -3.9488000e-01 1.5496000e-01 1.2113000e-02 /
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CH2C[OH]cHCH3+H(+m)=CH3C[O]cHCH3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -0.19992958293743612
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6528000e+00 -1.5156000e+00 -3.2588000e-02 /
CHEB / 3.7590000e+00 8.4947000e-01 -4.4291000e-02 /
CHEB / 4.9095000e-01 5.5809000e-01 6.5488000e-04 /
CHEB / -2.5880000e-01 2.4206000e-01 3.4665000e-02 /
CHEB / -2.5372000e-01 2.3113000e-02 3.8267000e-02 /

C4H7-22+OH(+m)=MEKenol(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     O_pri_rad           deltaHrxn(T=298K) = -
109.03858878266654 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1878000e+01 6.1255000e-01 -9.1153000e-02 /
CHEB / -1.6945000e+00 1.0592000e+00 -1.3041000e-01 /
CHEB / -1.2736000e+00 7.0064000e-01 -3.9708000e-02 /
CHEB / -8.3600000e-01 3.5095000e-01 1.9961000e-02 /
CHEB / -5.0922000e-01 1.2259000e-01 3.1803000e-02 /

C4H7-22+OH(+m)=CH3+CH3CHcOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -5.499578877674097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8763000e+00 -1.2992000e+00 -6.3828000e-02 /
CHEB / 2.3338000e+00 1.0575000e+00 -4.0091000e-02 /
CHEB / 3.2887000e-01 4.2368000e-01 6.5878000e-02 /
CHEB / -1.3672000e-01 -3.8489000e-04 6.7443000e-02 /
CHEB / -1.0271000e-01 -1.1434000e-01 1.2391000e-02 /

C4H7-22+OH(+m)=CH2C[OH]cHCH3+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -20.848090996581313
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8748000e+00 -1.3709000e+00 -5.5396000e-02 /
CHEB / 1.5822000e+00 1.0022000e+00 -4.7344000e-02 /
CHEB / 1.7232000e-01 4.8822000e-01 4.3645000e-02 /
CHEB / -1.6066000e-01 7.9948000e-02 6.5661000e-02 /
CHEB / -1.3353000e-01 -8.6908000e-02 2.9505000e-02 /

C4H7-22+OH(+m)=CH3C[OH]cH+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -6.829459805150272
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0594000e+01 -1.3071000e+00 -6.2533000e-02 /
CHEB / 2.0609000e+00 1.0528000e+00 -4.1000000e-02 /
CHEB / 2.7448000e-01 4.3181000e-01 6.3267000e-02 /
CHEB / -1.5298000e-01 7.2825000e-03 6.7598000e-02 /
CHEB / -1.1207000e-01 -1.1308000e-01 1.4356000e-02 /
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C4H7-22+OH(+m)=CH3C[OH]CHcH2+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -20.848090996581313
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8748000e+00 -1.3709000e+00 -5.5396000e-02 /
CHEB / 1.5822000e+00 1.0022000e+00 -4.7344000e-02 /
CHEB / 1.7232000e-01 4.8822000e-01 4.3645000e-02 /
CHEB / -1.6066000e-01 7.9948000e-02 6.5661000e-02 /
CHEB / -1.3353000e-01 -8.6908000e-02 2.9505000e-02 /

C4H7-22+OH(+m)=CH3C[O]cHCH3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -21.04802057951874
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9749000e+00 -1.3689000e+00 -5.5535000e-02 /
CHEB / 1.2717000e+00 1.0042000e+00 -4.7130000e-02 /
CHEB / 9.3063000e-02 4.8671000e-01 4.4235000e-02 /
CHEB / -1.8911000e-01 7.7400000e-02 6.5783000e-02 /
CHEB / -1.4425000e-01 -8.8223000e-02 2.9039000e-02 /

CH3C[OH]cH+CH3(+m)=MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination exact:
Cd_pri_rad     C_methyl       deltaHrxn(T=298K) = -102.20912897751626
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3211000e+01 4.6556000e-01 -5.7168000e-02 /
CHEB / -1.3209000e+00 8.3593000e-01 -9.0184000e-02 /
CHEB / -1.0628000e+00 6.0340000e-01 -3.7735000e-02 /
CHEB / -7.2441000e-01 3.4278000e-01 7.4891000e-03 /
CHEB / -4.6660000e-01 1.4241000e-01 2.5700000e-02 /

CH3C[OH]cH+CH3(+m)=CH2C[OH]cHCH3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -14.018631191431034
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0525000e+01 -1.4310000e+00 -4.3195000e-02 /
CHEB / 2.1888000e+00 9.5180000e-01 -4.8152000e-02 /
CHEB / 3.2635000e-01 5.3309000e-01 2.1909000e-02 /
CHEB / -1.5917000e-01 1.4591000e-01 5.5284000e-02 /
CHEB / -1.5773000e-01 -5.6738000e-02 3.8106000e-02 /

CH3C[OH]cH+CH3(+m)=CH3C[OH]CHcH2+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -14.018631191431034
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0525000e+01 -1.4310000e+00 -4.3195000e-02 /
CHEB / 2.1888000e+00 9.5180000e-01 -4.8152000e-02 /
CHEB / 3.2635000e-01 5.3309000e-01 2.1909000e-02 /
CHEB / -1.5917000e-01 1.4591000e-01 5.5284000e-02 /
CHEB / -1.5773000e-01 -5.6738000e-02 3.8106000e-02 /
```

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CH3C[OH]cH+CH3(+m)=CH3C[O]cHCH3+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -14.218560774368477
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6128000e+00 -1.4286000e+00 -4.3379000e-02 /
CHEB / 1.8890000e+00 9.5449000e-01 -4.8071000e-02 /
CHEB / 2.4682000e-01 5.3195000e-01 2.2545000e-02 /
CHEB / -1.8876000e-01 1.4295000e-01 5.5678000e-02 /
CHEB / -1.6835000e-01 -5.8836000e-02 3.7822000e-02 /

CH3C[OH]cCH3+H(+m)=MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
108.98831121920662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1927000e+01 5.9480000e-01 -8.6644000e-02 /
CHEB / -1.6696000e+00 1.0340000e+00 -1.2579000e-01 /
CHEB / -1.2456000e+00 6.9119000e-01 -3.9990000e-02 /
CHEB / -8.1788000e-01 3.5104000e-01 1.8464000e-02 /
CHEB / -4.9807000e-01 1.2481000e-01 3.1376000e-02 /

CH3C[OH]cCH3+H(+m)=CH3+CH3CHcOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = -5.449301314214182
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8175000e+00 -1.3054000e+00 -6.2334000e-02 /
CHEB / 2.4169000e+00 1.0550000e+00 -4.1006000e-02 /
CHEB / 3.4331000e-01 4.2999000e-01 6.3689000e-02 /
CHEB / -1.3152000e-01 4.5275000e-03 6.7600000e-02 /
CHEB / -9.6634000e-02 -1.1398000e-01 1.3796000e-02 /

CH3C[OH]cCH3+H(+m)=CH2C[OH]cHCH3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -20.797813433121398
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8578000e+00 -1.3781000e+00 -5.3684000e-02 /
CHEB / 1.6228000e+00 9.9748000e-01 -4.7775000e-02 /
CHEB / 1.9268000e-01 4.9431000e-01 4.0911000e-02 /
CHEB / -1.5351000e-01 8.7007000e-02 6.4803000e-02 /
CHEB / -1.2865000e-01 -8.4499000e-02 3.0759000e-02 /

CH3C[OH]cCH3+H(+m)=C4H7-22+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol)      deltaHrxn(T=298K) = 0.05027756345991108
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9326000e+00 -1.2661000e+00 -7.0389000e-02 /
CHEB / 3.0093000e+00 1.0721000e+00 -3.5138000e-02 /
CHEB / 3.4446000e-01 3.8865000e-01 7.6740000e-02 /
CHEB / -1.2144000e-01 -2.7891000e-02 6.5529000e-02 /
CHEB / -8.2502000e-02 -1.1609000e-01 4.3690000e-03 /
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CH3C[OH]cCH3+H(+m)=CH3C[OH]cH+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -6.779182241690357
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0541000e+01 -1.3134000e+00 -6.0989000e-02 /
CHEB / 2.1359000e+00 1.0502000e+00 -4.1897000e-02 /
CHEB / 2.9180000e-01 4.3815000e-01 6.1009000e-02 /
CHEB / -1.4841000e-01 1.2420000e-02 6.7664000e-02 /
CHEB / -1.0603000e-01 -1.1255000e-01 1.5769000e-02 /

CH3C[OH]cCH3+H(+m)=CH3C[OH]CHcH2+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -20.797813433121398
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8578000e+00 -1.3781000e+00 -5.3684000e-02 /
CHEB / 1.6228000e+00 9.9748000e-01 -4.7775000e-02 /
CHEB / 1.9268000e-01 4.9431000e-01 4.0911000e-02 /
CHEB / -1.5351000e-01 8.7007000e-02 6.4803000e-02 /
CHEB / -1.2865000e-01 -8.4499000e-02 3.0759000e-02 /

CH3C[OH]cCH3+H(+m)=CH3C[O]cHCH3+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -20.99774301605884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9568000e+00 -1.3760000e+00 -5.3829000e-02 /
CHEB / 1.3132000e+00 9.9952000e-01 -4.7576000e-02 /
CHEB / 1.1343000e-01 4.9282000e-01 4.1513000e-02 /
CHEB / -1.8205000e-01 8.4401000e-02 6.4957000e-02 /
CHEB / -1.3936000e-01 -8.5893000e-02 3.0307000e-02 /

CH3C[OH]CHcH2+H(+m)=MEKenol(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
88.19049778608522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3374000e+01 2.7293000e-01 -2.3683000e-02 /
CHEB / -9.2526000e-01 5.0839000e-01 -4.0314000e-02 /
CHEB / -7.2828000e-01 4.0872000e-01 -2.2647000e-02 /
CHEB / -5.5365000e-01 2.7884000e-01 -2.5502000e-03 /
CHEB / -3.9488000e-01 1.5496000e-01 1.2113000e-02 /

CH3C[OH]CHcH2+H(+m)=CH2C[OH]cHCH3+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6215000e+00 -1.5186000e+00 -3.2313000e-02 /
CHEB / 3.9914000e+00 8.4534000e-01 -4.4144000e-02 /
CHEB / 5.8860000e-01 5.5801000e-01 1.0190000e-04 /
CHEB / -2.2851000e-01 2.4501000e-01 3.3932000e-02 /
CHEB / -2.4319000e-01 2.6426000e-02 3.8002000e-02 /
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CH3C[OH]CHcH2+H(+m)=CH3C[O]cHCH3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (MEKenol) deltaHrxn(T=298K) = -0.19992958293743612
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6528000e+00 -1.5156000e+00 -3.2588000e-02 /
CHEB / 3.7590000e+00 8.4947000e-01 -4.4291000e-02 /
CHEB / 4.9095000e-01 5.5809000e-01 6.5488000e-04 /
CHEB / -2.5880000e-01 2.4206000e-01 3.4665000e-02 /
CHEB / -2.5372000e-01 2.3113000e-02 3.8267000e-02 /

CH3C[O]cHCH3+H(+m)=MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (MEKenol) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     H_rad          deltaHrxn(T=298K) = -
87.99056820314779 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2168000e+01 2.7886000e-01 -2.4522000e-02 /
CHEB / -8.4437000e-01 5.1889000e-01 -4.1664000e-02 /
CHEB / -7.6944000e-01 4.1585000e-01 -2.3242000e-02 /
CHEB / -5.8243000e-01 2.8209000e-01 -2.4486000e-03 /
CHEB / -4.1352000e-01 1.5528000e-01 1.2496000e-02 /

!PDepNetwork MEKenol2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     MEKenol2          -43.57      82.42 24.3  30.12 35.09 39.31 46.17
      51.2  58.73 null
!     cHC[OH]C2H5       15.53 83.81 24.11 29.37 33.73 37.39 43.35 47.71
      54.2  null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3O-2           28.54 64.12 14.36 16.86 18.74 20.19 22.32 23.9
      26.53
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H7-12           56.79 75.42 20.23 24.88 29.1  32.76 38.62 43.06
      49.99 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2C[OH]CH2       -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26
      40.88 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CH2C[OH]cHCH3           -10.58      79.45 23.81 29.21 33.69 37.49
      43.71 48.21 54.89 null
!     CH2C[OH]CH2cH2          5.43  85.83 23.53 28.76 33.18 36.91 43.01
      47.46 54.07 null
!     cH2C[O]C2H5       -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!Here are the path reactions and their high-P limit kinetics:
!     cHC[OH]C2H5+H=MEKenol2        5.3600000e+14      0.00000
9.8000000e+02
```

```
!     C2H3O-2+C2H5=MEKenol2   1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7-12+OH=MEKenol2     1.4157154e+13      -0.15000
2.9166667e+02
!     CH2C[OH]CH2+CH3=MEKenol2      2.4874006e+15      -0.90000
2.5000000e+02
!     CH2C[OH]cHCH3+H=MEKenol2      5.0000000e+13      0.00000
0.0000000e+00
!     CH2C[OH]CH2cH2+H=MEKenol2     1.0000000e+14      0.00000
0.0000000e+00
!     cH2C[O]C2H5+H=MEKenol2        1.4157154e+13      -0.15000
2.9166667e+02

cHC[OH]C2H5+H(+m)=MEKenol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -111.1880866510646
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1623000e+01 3.0893000e+00 -9.9050000e-01 /
CHEB / -1.6364000e+00 9.0841000e-01 2.8549000e-01 /
CHEB / -1.4100000e+00 5.7674000e-01 1.3462000e-01 /
CHEB / -7.9264000e-01 1.8768000e-01 6.9837000e-02 /
CHEB / -4.3704000e-01 2.8188000e-02 3.0728000e-02 /

cHC[OH]C2H5+H(+m)=C2H3O-2+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -9.658616872218406
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1207000e+01 -6.1392000e-01 -2.2185000e-01 /
CHEB / 2.3545000e+00 6.0240000e-01 1.8375000e-01 /
CHEB / 5.9435000e-01 1.1085000e-01 7.0531000e-02 /
CHEB / 8.5403000e-02 -5.2376000e-02 -2.4020000e-03 /
CHEB / -1.2794000e-02 -4.2264000e-02 -2.0439000e-02 /

cHC[OH]C2H5+H(+m)=C4H7-12+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -2.149497870150821
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3604000e+00 -5.7165000e-01 -2.1235000e-01 /
CHEB / 3.4502000e+00 5.8577000e-01 1.8425000e-01 /
CHEB / 7.5520000e-01 7.4427000e-02 6.2489000e-02 /
CHEB / 1.1028000e-01 -5.1099000e-02 -8.5022000e-03 /
CHEB / 3.0338000e-03 -3.6713000e-02 -1.9988000e-02 /

cHC[OH]C2H5+H(+m)=CH2C[OH]CH2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
35.086286643207025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3928000e+01 -6.0747000e-01 -2.4838000e-01 /
CHEB / 6.0321000e-01 5.3318000e-01 1.9136000e-01 /
CHEB / 4.0035000e-02 1.6675000e-01 8.3325000e-02 /
CHEB / -4.7779000e-02 -2.4751000e-02 9.5093000e-03 /
CHEB / -5.3399000e-02 -4.7048000e-02 -1.7149000e-02 /
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```
cHC[OH]C2H5+H(+m)=CH2C[OH]cHCH3+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
26.107328925217807 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1248000e+01 -6.1859000e-01 -2.4115000e-01 /
CHEB / 1.9087000e+00 5.5646000e-01 1.8848000e-01 /
CHEB / 4.3114000e-01 1.5883000e-01 8.0213000e-02 /
CHEB / 8.2651000e-02 -3.2670000e-02 6.9312000e-03 /
CHEB / -5.8167000e-03 -4.7804000e-02 -1.8115000e-02 /

cHC[OH]C2H5+H(+m)=CH2C[OH]CH2cH2+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
10.09890128422061 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0343000e+01 -6.1605000e-01 -2.2333000e-01 /
CHEB / 2.8975000e+00 6.0024000e-01 1.8413000e-01 /
CHEB / 7.4110000e-01 1.1586000e-01 7.1271000e-02 /
CHEB / 1.4234000e-01 -5.1597000e-02 -1.6326000e-03 /
CHEB / 9.6024000e-03 -4.3129000e-02 -2.0342000e-02 /

cHC[OH]C2H5+H(+m)=cH2C[O]C2H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -23.407587312915602
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0939000e+01 -6.2161000e-01 -2.3788000e-01 /
CHEB / 1.8222000e+00 5.6644000e-01 1.8741000e-01 /
CHEB / 4.2728000e-01 1.5362000e-01 7.8751000e-02 /
CHEB / 7.5994000e-02 -3.6551000e-02 5.5980000e-03 /
CHEB / -1.0387000e-02 -4.7778000e-02 -1.8588000e-02 /

C2H3O-2+C2H5(+m)=MEKenol2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_rad/H2/Cs         deltaHrxn(T=298K) = -
101.52946977884619 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1274000e+01 1.5392000e+00 -4.7027000e-01 /
CHEB / -1.9692000e+00 1.1779000e+00 4.2473000e-02 /
CHEB / -1.3144000e+00 6.5518000e-01 5.9053000e-02 /
CHEB / -7.6063000e-01 2.3310000e-01 6.9184000e-02 /
CHEB / -4.3645000e-01 5.0125000e-02 4.0983000e-02 /

C2H3O-2+C2H5(+m)=CH2C[OH]CH2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
25.427669770988622 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2063000e+01 -9.5021000e-01 -2.1068000e-01 /
CHEB / 4.6166000e-01 8.1079000e-01 1.1127000e-01 /
CHEB / 9.8446000e-02 2.6198000e-01 9.8571000e-02 /
CHEB / -6.4284000e-02 -1.7078000e-02 4.0467000e-02 /
CHEB / -7.5241000e-02 -6.4079000e-02 -7.9663000e-03 /
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C2H3O-2+C2H5(+m)=CH2C[OH]cHCH3+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
16.448712052999404 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2101000e+00 -9.3942000e-01 -2.0308000e-01 /
CHEB / 1.8980000e+00 8.2932000e-01 1.0926000e-01 /
CHEB / 5.0918000e-01 2.3959000e-01 9.8981000e-02 /
CHEB / 6.1978000e-02 -3.1816000e-02 3.5531000e-02 /
CHEB / -2.8693000e-02 -6.5109000e-02 -1.2165000e-02 /

C2H3O-2+C2H5(+m)=cH2C[O]C2H5+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -13.7489704406972
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8107000e+00 -9.3095000e-01 -2.0041000e-01 /
CHEB / 1.8884000e+00 8.3603000e-01 1.0923000e-01 /
CHEB / 5.1193000e-01 2.2644000e-01 9.9459000e-02 /
CHEB / 5.1638000e-02 -3.8334000e-02 3.2791000e-02 /
CHEB / -3.3622000e-02 -6.4621000e-02 -1.4171000e-02 /

C4H7-12+OH(+m)=MEKenol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     O_pri_rad           deltaHrxn(T=298K) = -
109.03858878091377 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0241000e+01 2.6932000e+00 -8.8023000e-01 /
CHEB / -1.9627000e+00 9.8289000e-01 2.4311000e-01 /
CHEB / -1.4192000e+00 6.0251000e-01 1.1754000e-01 /
CHEB / -8.0500000e-01 1.9894000e-01 6.9379000e-02 /
CHEB / -4.5052000e-01 3.2539000e-02 3.2782000e-02 /

C4H7-12+OH(+m)=C2H3O-2+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -7.509119002067582
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2920000e+00 -6.6754000e-01 -2.2052000e-01 /
CHEB / 2.2124000e+00 6.5590000e-01 1.7523000e-01 /
CHEB / 5.8586000e-01 1.1705000e-01 7.6798000e-02 /
CHEB / 5.8434000e-02 -5.4378000e-02 7.7983000e-04 /
CHEB / -3.0775000e-02 -4.4905000e-02 -2.1160000e-02 /

C4H7-12+OH(+m)=CH2C[OH]CH2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -32.9367887730562
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2175000e+01 -6.7872000e-01 -2.4964000e-01 /
CHEB / 3.1774000e-01 5.9234000e-01 1.8381000e-01 /
CHEB / 2.5612000e-02 1.8621000e-01 8.8325000e-02 /
CHEB / -6.8706000e-02 -2.4252000e-02 1.5224000e-02 /
CHEB / -7.1101000e-02 -5.1001000e-02 -1.6176000e-02 /
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C4H7-12+OH(+m)=CH2C[OH]cHCH3+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -23.957831055066983
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4615000e+00 -6.8672000e-01 -2.4117000e-01 /
CHEB / 1.6464000e+00 6.1558000e-01 1.8022000e-01 /
CHEB / 4.2138000e-01 1.7573000e-01 8.5351000e-02 /
CHEB / 6.1374000e-02 -3.3485000e-02 1.2178000e-02 /
CHEB / -2.3757000e-02 -5.1797000e-02 -1.7621000e-02 /

C4H7-12+OH(+m)=CH2C[OH]CH2cH2+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -7.949403414069785
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4405000e+00 -6.7157000e-01 -2.2193000e-01 /
CHEB / 2.7411000e+00 6.5532000e-01 1.7543000e-01 /
CHEB / 7.3478000e-01 1.2265000e-01 7.7492000e-02 /
CHEB / 1.1559000e-01 -5.3716000e-02 1.7477000e-03 /
CHEB / -8.5008000e-03 -4.5847000e-02 -2.1010000e-02 /

C4H7-12+OH(+m)=cH2C[O]C2H5+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2)    deltaHrxn(T=298K) = -21.258089442764778
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1360000e+00 -6.8809000e-01 -2.3745000e-01 /
CHEB / 1.5731000e+00 6.2541000e-01 1.7891000e-01 /
CHEB / 4.1947000e-01 1.6911000e-01 8.4012000e-02 /
CHEB / 5.4239000e-02 -3.7919000e-02 1.0605000e-02 /
CHEB / -2.8467000e-02 -5.1689000e-02 -1.8318000e-02 /

CH2C[OH]CH2+CH3(+m)=MEKenol2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_methyl       deltaHrxn(T=298K) = -
76.10180000785758 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2231000e+01 3.6606000e-01 -3.2181000e-02 /
CHEB / -1.3145000e+00 6.6269000e-01 -4.8279000e-02 /
CHEB / -9.3345000e-01 4.8961000e-01 -1.2501000e-02 /
CHEB / -6.1390000e-01 2.8955000e-01 1.8856000e-02 /
CHEB / -4.0061000e-01 1.2852000e-01 3.1169000e-02 /

CH2C[OH]cHCH3+H(+m)=MEKenol2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
85.08075772584678 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3111000e+01 4.9757000e-01 -6.1080000e-02 /
CHEB / -1.3046000e+00 8.5994000e-01 -7.9168000e-02 /
CHEB / -9.7399000e-01 5.7457000e-01 -9.0141000e-03 /
CHEB / -6.5328000e-01 2.9485000e-01 3.4769000e-02 /
CHEB / -4.0991000e-01 1.0782000e-01 3.9970000e-02 /
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CH2C[OH]cHCH3+H(+m)=CH2C[OH]CH2+CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
8.978957717989218 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1764000e+01 -1.3567000e+00 -6.9156000e-02 /
CHEB / 1.8131000e+00 9.9339000e-01 -5.2059000e-02 /
CHEB / 3.1197000e-01 4.5793000e-01 5.4452000e-02 /
CHEB / -1.2879000e-01 7.4208000e-02 7.0855000e-02 /
CHEB / -1.1492000e-01 -6.8680000e-02 2.9483000e-02 /

CH2C[OH]CH2cH2+H(+m)=MEKenol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -101.08918536684398
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2574000e+01 1.4118000e+00 -4.1790000e-01 /
CHEB / -1.8169000e+00 1.1896000e+00 1.4684000e-02 /
CHEB / -1.2745000e+00 6.5697000e-01 5.2572000e-02 /
CHEB / -7.4940000e-01 2.3763000e-01 6.8936000e-02 /
CHEB / -4.3078000e-01 5.3170000e-02 4.1904000e-02 /

CH2C[OH]CH2cH2+H(+m)=C2H3O-2+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) =
0.44028441200221025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4718000e+00 -8.4010000e-01 -2.0163000e-01 /
CHEB / 3.4015000e+00 8.1368000e-01 1.2740000e-01 /
CHEB / 6.2949000e-01 1.4871000e-01 9.9058000e-02 /
CHEB / 4.1210000e-02 -5.2342000e-02 1.3912000e-02 /
CHEB / -2.7103000e-02 -5.6489000e-02 -2.0925000e-02 /

CH2C[OH]CH2cH2+H(+m)=CH2C[OH]CH2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
24.98738535898641 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3219000e+01 -9.8933000e-01 -1.9974000e-01 /
CHEB / 6.3586000e-01 8.4051000e-01 9.5553000e-02 /
CHEB / 1.3187000e-01 2.7374000e-01 9.8894000e-02 /
CHEB / -6.0141000e-02 -1.4908000e-02 4.4414000e-02 /
CHEB / -7.2539000e-02 -6.5743000e-02 -6.1764000e-03 /

CH2C[OH]CH2cH2+H(+m)=CH2C[OH]cHCH3+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
16.00842764099719 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0343000e+01 -9.7482000e-01 -1.9334000e-01 /
CHEB / 2.0921000e+00 8.5775000e-01 9.4688000e-02 /
CHEB / 5.4420000e-01 2.4936000e-01 1.0019000e-01 /
CHEB / 6.5210000e-02 -3.0599000e-02 3.9180000e-02 /
CHEB / -2.6024000e-02 -6.6866000e-02 -1.0895000e-02 /
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CH2C[OH]CH2cH2+H(+m)=cH2C[O]C2H5+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
13.308686028694986 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9304000e+00 -9.6439000e-01 -1.9134000e-01 /
CHEB / 2.0945000e+00 8.6362000e-01 9.5320000e-02 /
CHEB / 5.4701000e-01 2.3513000e-01 1.0109000e-01 /
CHEB / 5.4232000e-02 -3.7458000e-02 3.6228000e-02 /
CHEB / -3.0897000e-02 -6.6333000e-02 -1.3148000e-02 /

cH2C[O]C2H5+H(+m)=MEKenol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (MEKenol2) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     H_rad          deltaHrxn(T=298K) = -
87.780499338149 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1918000e+01 5.8131000e-01 -8.5013000e-02 /
CHEB / -1.3854000e+00 9.5922000e-01 -9.2878000e-02 /
CHEB / -1.0575000e+00 6.0486000e-01 -2.2650000e-03 /
CHEB / -6.8570000e-01 2.8903000e-01 4.3821000e-02 /
CHEB / -4.2065000e-01 9.6901000e-02 4.2514000e-02 /

cH2C[O]C2H5+H(+m)=CH2C[OH]CH2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
11.67869933029143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0994000e+01 -1.3179000e+00 -8.1235000e-02 /
CHEB / 1.5063000e+00 1.0028000e+00 -4.4192000e-02 /
CHEB / 2.5620000e-01 4.2641000e-01 6.7497000e-02 /
CHEB / -1.1864000e-01 5.0095000e-02 7.1431000e-02 /
CHEB / -1.0950000e-01 -7.3147000e-02 2.2981000e-02 /

cH2C[O]C2H5+H(+m)=CH2C[OH]cHCH3+H(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (MEKenol2)     deltaHrxn(T=298K) = -
2.699741612302212 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7213000e+00 -1.2665000e+00 -9.2560000e-02 /
CHEB / 3.3567000e+00 1.0210000e+00 -3.4163000e-02 /
CHEB / 6.3484000e-01 3.8049000e-01 8.3397000e-02 /
CHEB / -5.3493000e-03 1.4811000e-02 6.8746000e-02 /
CHEB / -5.5688000e-02 -8.0670000e-02 1.2901000e-02 /

!PDepNetwork sC4H8O
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sC4H8O            -39.25      81.78 24.22 30.55 35.99 40.19 47.0
      51.9  58.85 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
```

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!     cH2CH[OH]C2H3           9.75  85.19 23.45 29.19 34.08 37.79 43.84
      48.16 54.19 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3C[OH]CHcH2           -10.58      79.45 23.81 29.21 33.69 37.49
      43.71 48.21 54.89 null
!     CH3CH[OH]cCH2           17.65 83.59 23.88 29.34 34.05 37.67 43.66
      47.99 54.09 null
!     CH3CH[OH]CHcH           19.85 83.17 24.03 29.8  34.63 38.27 44.18
      48.41 54.32 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H5O-enol2=sC4H8O        6.8000000e+14      -0.68000
0.0000000e+00
!     cH2CH[OH]C2H3+H=sC4H8O        1.0000000e+14      0.00000
0.0000000e+00
!     C2H5O-2+C2H3=sC4H8O     1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7-24+OH=sC4H8O       1.4157154e+13      -0.15000
2.9166667e+02
!     CH3C[OH]CHcH2+H=sC4H8O        5.0000000e+13      0.00000
0.0000000e+00
!     CH3CH[OH]cCH2+H=sC4H8O        1.4157154e+13      -0.15000
2.9166667e+02
!     CH3CH[OH]CHcH+H=sC4H8O        5.3600000e+14      0.00000
9.8000000e+02
!     CH3CH[o]C2H3+H=sC4H8O         1.4157154e+13      -0.15000
2.9166667e+02
!     C4H6-13+H2O=sC4H8O      6.5200000e+01      2.92000
5.0700000e+04

CH3+C3H5O-enol2(+m)=sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) C_methyl     C_rad/H/OneDeO          deltaHrxn(T=298K) = -
73.11207307528315 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2377000e+01 4.4917000e-01 -4.4766000e-02 /
CHEB / -1.7606000e+00 8.1151000e-01 -6.9520000e-02 /
CHEB / -1.1845000e+00 5.9629000e-01 -2.5305000e-02 /
CHEB / -8.1634000e-01 3.5008000e-01 1.3175000e-02 /
CHEB / -5.4587000e-01 1.5456000e-01 2.8611000e-02 /
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CH3+C3H5O-enol2(+m)=C4H6-13+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -63.373346038141264
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8409000e+00 -1.4520000e+00 -4.4879000e-02 /
CHEB / 2.5017000e+00 9.2457000e-01 -5.2073000e-02 /
CHEB / 4.6326000e-01 5.3713000e-01 1.8329000e-02 /
CHEB / -1.1049000e-01 1.7268000e-01 5.4789000e-02 /
CHEB / -1.4005000e-01 -2.9866000e-02 4.2371000e-02 /

cH2CH[OH]C2H3+H(+m)=sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -101.08918551224698
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1979000e+01 2.1688000e+00 -6.7777000e-01 /
CHEB / -2.5221000e+00 1.4327000e+00 6.8829000e-02 /
CHEB / -1.6970000e+00 7.9710000e-01 5.9021000e-02 /
CHEB / -1.0229000e+00 3.1482000e-01 4.7348000e-02 /
CHEB / -6.0290000e-01 9.9107000e-02 1.9496000e-02 /

cH2CH[OH]C2H3+H(+m)=CH3+C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -27.97711243696383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3537000e+01 -8.1259000e-01 -2.3118000e-01 /
CHEB / 3.9191000e-01 7.3453000e-01 1.5652000e-01 /
CHEB / 8.8193000e-02 2.0467000e-01 9.6106000e-02 /
CHEB / -4.8304000e-02 -3.8823000e-02 2.1326000e-02 /
CHEB / -5.1913000e-02 -6.4198000e-02 -1.8387000e-02 /

cH2CH[OH]C2H3+H(+m)=C2H5O-2+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -2.5694172581219448
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0241000e+01 -7.2978000e-01 -2.0664000e-01 /
CHEB / 2.5887000e+00 7.5093000e-01 1.5843000e-01 /
CHEB / 5.8230000e-01 9.4713000e-02 8.5249000e-02 /
CHEB / 4.1563000e-02 -6.6759000e-02 -3.2229000e-03 /
CHEB / -1.7063000e-02 -4.9152000e-02 -2.4776000e-02 /

cH2CH[OH]C2H3+H(+m)=C4H7-24+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -18.377915085000463
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1409000e+01 -8.0966000e-01 -2.1906000e-01 /
CHEB / 1.0613000e+00 7.6070000e-01 1.5146000e-01 /
CHEB / 3.1815000e-01 1.8054000e-01 9.3197000e-02 /
CHEB / 1.3770000e-02 -5.4182000e-02 1.5558000e-02 /
CHEB / -3.2523000e-02 -6.3259000e-02 -2.1344000e-02 /
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cH2CH[OH]C2H3+H(+m)=CH3C[OH]CHcH2+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -20.328035640967975
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1053000e+01 -8.1210000e-01 -2.2232000e-01 /
CHEB / 1.4714000e+00 7.5379000e-01 1.5260000e-01 /
CHEB / 4.1381000e-01 1.8887000e-01 9.3972000e-02 /
CHEB / 5.4345000e-02 -4.9712000e-02 1.7400000e-02 /
CHEB / -1.5125000e-02 -6.3952000e-02 -2.0457000e-02 /

cH2CH[OH]C2H3+H(+m)=C4H6-13+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -91.3504584751051
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1137000e+01 -7.9930000e-01 -2.4776000e-01 /
CHEB / 1.4184000e+00 7.0094000e-01 1.6588000e-01 /
CHEB / 2.7327000e-01 2.1858000e-01 1.0066000e-01 /
CHEB / 2.0356000e-02 -2.4434000e-02 2.6445000e-02 /
CHEB / -2.1138000e-02 -6.2371000e-02 -1.5698000e-02 /

C2H5O-2+C2H3(+m)=sC4H8O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/CsO     Cd_pri_rad           deltaHrxn(T=298K) = -
98.51976825412504 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0681000e+01 2.0031000e+00 -6.1713000e-01 /
CHEB / -2.4571000e+00 1.4477000e+00 3.9872000e-02 /
CHEB / -1.7117000e+00 8.0167000e-01 5.1281000e-02 /
CHEB / -1.0344000e+00 3.1823000e-01 4.7778000e-02 /
CHEB / -6.1696000e-01 1.0029000e-01 2.1024000e-02 /

C2H5O-2+C2H3(+m)=CH3+C3H5O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -25.407695178841884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2071000e+01 -8.5223000e-01 -2.2429000e-01 /
CHEB / 4.6635000e-01 7.6718000e-01 1.4438000e-01 /
CHEB / 6.3315000e-02 2.1597000e-01 9.8072000e-02 /
CHEB / -6.8725000e-02 -3.8295000e-02 2.5294000e-02 /
CHEB / -7.0309000e-02 -6.6651000e-02 -1.7312000e-02 /

C2H5O-2+C2H3(+m)=C4H7-24+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -15.808497826878519
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9150000e+00 -8.4517000e-01 -2.1259000e-01 /
CHEB / 1.1595000e+00 7.9198000e-01 1.3991000e-01 /
CHEB / 2.9597000e-01 1.8918000e-01 9.5839000e-02 /
CHEB / -7.5714000e-03 -5.4694000e-02 1.9029000e-02 /
CHEB / -5.0997000e-02 -6.5559000e-02 -2.0847000e-02 /
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C2H5O-2+C2H3(+m)=CH3C[OH]CHcH2+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -17.75861838284603
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5674000e+00 -8.4891000e-01 -2.1568000e-01 /
CHEB / 1.5614000e+00 7.8553000e-01 1.4084000e-01 /
CHEB / 3.9104000e-01 1.9837000e-01 9.6393000e-02 /
CHEB / 3.3396000e-02 -4.9962000e-02 2.1040000e-02 /
CHEB / -3.3588000e-02 -6.6341000e-02 -1.9789000e-02 /

C2H5O-2+C2H3(+m)=C4H6-13+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -88.78104121698316
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6977000e+00 -8.4308000e-01 -2.4080000e-01 /
CHEB / 1.4759000e+00 7.3498000e-01 1.5328000e-01 /
CHEB / 2.4456000e-01 2.3208000e-01 1.0214000e-01 /
CHEB / -1.2280000e-04 -2.2638000e-02 3.0857000e-02 /
CHEB / -3.9532000e-02 -6.4631000e-02 -1.4011000e-02 /

C4H7-24+OH(+m)=sC4H8O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     O_pri_rad         deltaHrxn(T=298K) = -
82.71127042724652 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1860000e+01 6.7421000e-01 -9.9787000e-02 /
CHEB / -1.8669000e+00 1.1288000e+00 -1.2111000e-01 /
CHEB / -1.3637000e+00 7.2519000e-01 -2.0963000e-02 /
CHEB / -9.1701000e-01 3.5954000e-01 3.2227000e-02 /
CHEB / -5.8467000e-01 1.3167000e-01 3.4979000e-02 /

C4H7-24+OH(+m)=CH3+C3H5O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -9.599197351963364
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1120000e+01 -1.2979000e+00 -7.8636000e-02 /
CHEB / 1.4340000e+00 1.0273000e+00 -3.9939000e-02 /
CHEB / 2.1566000e-01 4.1600000e-01 7.2007000e-02 /
CHEB / -1.4479000e-01 2.5389000e-02 7.0505000e-02 /
CHEB / -1.2032000e-01 -8.9803000e-02 1.7155000e-02 /

C4H7-24+OH(+m)=C4H6-13+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -72.97254339010463
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2622000e+00 -1.3504000e+00 -7.1209000e-02 /
CHEB / 2.0437000e+00 9.9250000e-01 -4.6780000e-02 /
CHEB / 3.6279000e-01 4.6289000e-01 5.5571000e-02 /
CHEB / -6.5270000e-02 7.8039000e-02 7.0419000e-02 /
CHEB / -9.5566000e-02 -7.1467000e-02 2.9426000e-02 /
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CH3C[OH]CHcH2+H(+m)=sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) C_rad/ODMustO     H_rad        deltaHrxn(T=298K) = -
80.761149871279 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2966000e+01 5.9481000e-01 -7.7518000e-02 /
CHEB / -1.7032000e+00 1.0306000e+00 -1.0602000e-01 /
CHEB / -1.2703000e+00 6.9263000e-01 -2.5096000e-02 /
CHEB / -8.7389000e-01 3.6112000e-01 2.6027000e-02 /
CHEB / -5.6448000e-01 1.3866000e-01 3.4222000e-02 /

CH3C[OH]CHcH2+H(+m)=CH3+C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -7.649076795995855
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1858000e+01 -1.3304000e+00 -6.8646000e-02 /
CHEB / 1.7746000e+00 1.0205000e+00 -4.6757000e-02 /
CHEB / 2.7095000e-01 4.4451000e-01 6.1191000e-02 /
CHEB / -1.4644000e-01 4.5660000e-02 7.0934000e-02 /
CHEB / -1.1760000e-01 -8.7588000e-02 2.3116000e-02 /

CH3C[OH]CHcH2+H(+m)=C4H7-24+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = 1.950120555967512
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8619000e+00 -1.2487000e+00 -8.9476000e-02 /
CHEB / 3.3446000e+00 1.0430000e+00 -3.0293000e-02 /
CHEB / 3.8869000e-01 3.6838000e-01 8.7034000e-02 /
CHEB / -9.2879000e-02 -8.7727000e-03 6.6881000e-02 /
CHEB / -8.5184000e-02 -9.3612000e-02 6.6591000e-03 /

CH3C[OH]CHcH2+H(+m)=C4H6-13+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -71.02242283413712
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0122000e+01 -1.3865000e+00 -6.0160000e-02 /
CHEB / 2.2678000e+00 9.7778000e-01 -5.1727000e-02 /
CHEB / 4.2748000e-01 4.9150000e-01 4.2492000e-02 /
CHEB / -6.1022000e-02 1.0569000e-01 6.7335000e-02 /
CHEB / -9.6443000e-02 -6.2983000e-02 3.4910000e-02 /

CH3CH[OH]cCH2+H(+m)=sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
108.98831131612143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4077000e+00 3.6456000e+00 -1.0973000e+00 /
CHEB / -2.6670000e+00 1.2380000e+00 2.5033000e-01 /
CHEB / -1.8343000e+00 7.2484000e-01 1.1689000e-01 /
CHEB / -1.0735000e+00 2.8267000e-01 4.6129000e-02 /
CHEB / -6.1932000e-01 9.0793000e-02 1.1065000e-02 /
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```
CH3CH[OH]cCH2+H(+m)=CH3+C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -35.87623824083827
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2386000e+01 -5.3815000e-01 -2.3787000e-01 /
CHEB / 1.8582000e-01 5.0082000e-01 1.9884000e-01 /
CHEB / 1.2536000e-02 1.2996000e-01 7.4008000e-02 /
CHEB / -4.4156000e-02 -3.7319000e-02 -1.6914000e-03 /
CHEB / -4.1015000e-02 -4.5795000e-02 -2.1011000e-02 /

CH3CH[OH]cCH2+H(+m)=cH2CH[OH]C2H3+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -7.899125803874433
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2277000e+00 -5.5031000e-01 -2.1173000e-01 /
CHEB / 2.6654000e+00 5.7163000e-01 1.9112000e-01 /
CHEB / 7.7018000e-01 7.2747000e-02 5.8130000e-02 /
CHEB / 1.5628000e-01 -6.1341000e-02 -1.2907000e-02 /
CHEB / 2.3170000e-02 -3.6940000e-02 -2.1224000e-02 /

CH3CH[OH]cCH2+H(+m)=C2H5O-2+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -10.468543061996385
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8372000e+00 -5.5319000e-01 -2.1315000e-01 /
CHEB / 1.6716000e+00 5.7097000e-01 1.9139000e-01 /
CHEB / 5.1600000e-01 7.7447000e-02 5.9200000e-02 /
CHEB / 7.2721000e-02 -6.1057000e-02 -1.2256000e-02 /
CHEB / -9.8152000e-03 -3.7968000e-02 -2.1360000e-02 /

CH3CH[OH]cCH2+H(+m)=C4H7-24+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -26.277040888874904
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0441000e+01 -5.5473000e-01 -2.3012000e-01 /
CHEB / 7.1884000e-01 5.3045000e-01 1.9562000e-01 /
CHEB / 2.1919000e-01 1.2096000e-01 7.0013000e-02 /
CHEB / 2.0958000e-02 -4.6056000e-02 -4.5023000e-03 /
CHEB / -2.0753000e-02 -4.5749000e-02 -2.1373000e-02 /

CH3CH[OH]cCH2+H(+m)=CH3C[OH]CHcH2+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -28.227161444842416
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0027000e+01 -5.5098000e-01 -2.3240000e-01 /
CHEB / 1.1745000e+00 5.2223000e-01 1.9643000e-01 /
CHEB / 3.2103000e-01 1.2436000e-01 7.1236000e-02 /
CHEB / 5.9926000e-02 -4.3376000e-02 -3.5952000e-03 /
CHEB / -3.6655000e-03 -4.5941000e-02 -2.1254000e-02 /
```

```
CH3CH[OH]cCH2+H(+m)=CH3CH[o]C2H3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -4.939387924082247
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1042000e+00 -5.3672000e-01 -2.0728000e-01 /
CHEB / 3.1493000e+00 5.6814000e-01 1.9048000e-01 /
CHEB / 8.5729000e-01 5.7889000e-02 5.4381000e-02 /
CHEB / 1.7086000e-01 -6.0745000e-02 -1.4906000e-02 /
CHEB / 3.0453000e-02 -3.3772000e-02 -2.0578000e-02 /

CH3CH[OH]cCH2+H(+m)=C4H6-13+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -99.24958427897954
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8183000e+00 -5.0642000e-01 -2.4662000e-01 /
CHEB / 1.3141000e+00 4.6376000e-01 2.0456000e-01 /
CHEB / 2.2496000e-01 1.3159000e-01 7.8138000e-02 /
CHEB / 2.7122000e-02 -3.0342000e-02 3.1259000e-04 /
CHEB / -9.8132000e-03 -4.4845000e-02 -2.1128000e-02 /

CH3CH[OH]CHcH+H(+m)=sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -111.18808679607585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0653000e+01 4.1951000e+00 -1.1964000e+00 /
CHEB / -2.4005000e+00 1.1593000e+00 2.8513000e-01 /
CHEB / -1.8447000e+00 6.9104000e-01 1.3146000e-01 /
CHEB / -1.0756000e+00 2.6994000e-01 4.5944000e-02 /
CHEB / -6.1670000e-01 8.7901000e-02 9.5246000e-03 /

CH3CH[OH]CHcH+H(+m)=CH3+C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -38.076013720792695
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4159000e+01 -4.5924000e-01 -2.2458000e-01 /
CHEB / 4.3792000e-01 4.3174000e-01 1.9480000e-01 /
CHEB / 1.8618000e-02 1.0902000e-01 6.5273000e-02 /
CHEB / -3.2236000e-02 -3.5457000e-02 -6.2913000e-03 /
CHEB / -3.1451000e-02 -3.9884000e-02 -2.0148000e-02 /

CH3CH[OH]CHcH+H(+m)=cH2CH[OH]C2H3+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -10.098901283828859
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0204000e+01 -4.8846000e-01 -2.0616000e-01 /
CHEB / 2.7438000e+00 5.0674000e-01 1.9196000e-01 /
CHEB / 7.6242000e-01 6.7256000e-02 5.0788000e-02 /
CHEB / 1.7503000e-01 -5.6741000e-02 -1.4956000e-02 /
CHEB / 3.3183000e-02 -3.3538000e-02 -1.9548000e-02 /
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CH3CH[OH]CHcH+H(+m)=C2H5O-2+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -12.66831854195081
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1799000e+01 -4.8964000e-01 -2.0735000e-01 /
CHEB / 1.7652000e+00 5.0490000e-01 1.9215000e-01 /
CHEB / 5.0705000e-01 7.0966000e-02 5.1800000e-02 /
CHEB / 9.0704000e-02 -5.6209000e-02 -1.4474000e-02 /
CHEB / 3.6150000e-04 -3.4379000e-02 -1.9692000e-02 /

CH3CH[OH]CHcH+H(+m)=C4H7-24+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -28.47681636882933
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2264000e+01 -4.7895000e-01 -2.1989000e-01 /
CHEB / 9.3717000e-01 4.6082000e-01 1.9364000e-01 /
CHEB / 2.1737000e-01 1.0339000e-01 6.1908000e-02 /
CHEB / 3.2778000e-02 -4.2465000e-02 -8.4330000e-03 /
CHEB / -1.0950000e-02 -4.0049000e-02 -2.0209000e-02 /

CH3CH[OH]CHcH+H(+m)=CH3C[OH]CHcH2+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -30.42693692479684
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1834000e+01 -4.7418000e-01 -2.2134000e-01 /
CHEB / 1.4039000e+00 4.5272000e-01 1.9389000e-01 /
CHEB / 3.2148000e-01 1.0569000e-01 6.2975000e-02 /
CHEB / 7.1613000e-02 -4.0280000e-02 -7.7244000e-03 /
CHEB / 6.0254000e-03 -4.0131000e-02 -2.0180000e-02 /

CH3CH[OH]CHcH+H(+m)=CH3CH[OH]cCH2+H(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -2.1997754799544325
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8932000e+00 -4.5892000e-01 -1.9462000e-01 /
CHEB / 3.6506000e+00 4.9847000e-01 1.8915000e-01 /
CHEB / 8.9934000e-01 3.4957000e-02 4.0942000e-02 /
CHEB / 1.8438000e-01 -5.4498000e-02 -1.8294000e-02 /
CHEB / 3.9903000e-02 -2.6442000e-02 -1.7535000e-02 /

CH3CH[OH]CHcH+H(+m)=CH3CH[o]C2H3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -7.1391634040366725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1301000e+00 -4.8220000e-01 -2.0210000e-01 /
CHEB / 3.1716000e+00 5.0989000e-01 1.9110000e-01 /
CHEB / 8.5716000e-01 5.4697000e-02 4.7422000e-02 /
CHEB / 1.9164000e-01 -5.7327000e-02 -1.6402000e-02 /
CHEB / 3.9619000e-02 -3.0706000e-02 -1.8966000e-02 /
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CH3CH[OH]CHcH+H(+m)=C4H6-13+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -101.44935975893397
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1544000e+01 -4.2503000e-01 -2.2902000e-01 /
CHEB / 1.5928000e+00 3.9538000e-01 1.9764000e-01 /
CHEB / 2.3942000e-01 1.0797000e-01 6.8286000e-02 /
CHEB / 4.0495000e-02 -3.0266000e-02 -5.0803000e-03 /
CHEB / 2.2503000e-05 -3.9042000e-02 -2.0558000e-02 /

CH3CH[o]C2H3+H(+m)=sC4H8O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
104.04892339203919 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0011000e+01 2.7169000e+00 -8.5950000e-01 /
CHEB / -2.4604000e+00 1.3679000e+00 1.5239000e-01 /
CHEB / -1.7700000e+00 7.7528000e-01 8.3379000e-02 /
CHEB / -1.0588000e+00 3.0335000e-01 4.6452000e-02 /
CHEB / -6.1652000e-01 9.5790000e-02 1.5364000e-02 /

CH3CH[o]C2H3+H(+m)=CH3+C3H5O-enol2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -30.93685031675603
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2105000e+01 -6.9680000e-01 -2.4307000e-01 /
CHEB / 4.2678000e-01 6.3726000e-01 1.8367000e-01 /
CHEB / 4.2613000e-02 1.7270000e-01 8.8572000e-02 /
CHEB / -5.9883000e-02 -3.9151000e-02 1.0574000e-02 /
CHEB / -5.3452000e-02 -5.6791000e-02 -2.0541000e-02 /

CH3CH[o]C2H3+H(+m)=cH2CH[OH]C2H3+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -2.9597378797921934
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5035000e+00 -6.5618000e-01 -2.1160000e-01 /
CHEB / 3.3197000e+00 6.8133000e-01 1.7642000e-01 /
CHEB / 8.0227000e-01 8.1734000e-02 7.3159000e-02 /
CHEB / 1.2430000e-01 -6.6035000e-02 -8.0938000e-03 /
CHEB / 1.2304000e-02 -4.3262000e-02 -2.3720000e-02 /

CH3CH[o]C2H3+H(+m)=C2H5O-2+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -5.529155137914145
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1462000e+00 -6.6497000e-01 -2.1238000e-01 /
CHEB / 2.2873000e+00 6.8648000e-01 1.7543000e-01 /
CHEB / 5.5474000e-01 8.7548000e-02 7.4551000e-02 /
CHEB / 4.1551000e-02 -6.6519000e-02 -6.9120000e-03 /
CHEB / -2.1252000e-02 -4.4416000e-02 -2.3895000e-02 /
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CH3CH[o]C2H3+H(+m)=C4H7-24+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -21.337652964792664
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0057000e+01 -7.0395000e-01 -2.3146000e-01 /
CHEB / 1.0338000e+00 6.6613000e-01 1.7835000e-01 /
CHEB / 2.6362000e-01 1.5560000e-01 8.4484000e-02 /
CHEB / 4.1589000e-03 -5.1623000e-02 6.1360000e-03 /
CHEB / -3.3726000e-02 -5.6269000e-02 -2.2105000e-02 /

CH3CH[o]C2H3+H(+m)=CH3C[OH]CHcH2+H(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #32 (sC4H8O) deltaHrxn(T=298K) = -23.287773520760176
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6752000e+00 -7.0321000e-01 -2.3472000e-01 /
CHEB / 1.4649000e+00 6.5825000e-01 1.7968000e-01 /
CHEB / 3.6150000e-01 1.6165000e-01 8.5662000e-02 /
CHEB / 4.3828000e-02 -4.7910000e-02 7.5410000e-03 /
CHEB / -1.6425000e-02 -5.6726000e-02 -2.1631000e-02 /

CH3CH[o]C2H3+H(+m)=C4H6-13+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O)      deltaHrxn(T=298K) = -94.3101963548973
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6326000e+00 -6.7364000e-01 -2.5778000e-01 /
CHEB / 1.4989000e+00 6.0085000e-01 1.9264000e-01 /
CHEB / 2.3898000e-01 1.8084000e-01 9.3715000e-02 /
CHEB / 9.3935000e-03 -2.8117000e-02 1.4404000e-02 /
CHEB / -2.2601000e-02 -5.5414000e-02 -1.9343000e-02 /

C4H6-13+H2O(+m)=sC4H8O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #32 (sC4H8O) High-P Limit: 1,3_Insertion_ROR estimate:
(Average:) Cd/H2_Cd/H/De     H_OH         deltaHrxn(T=298K) = -
9.738727037141889 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1244000e+01 2.9392000e-01 -1.9695000e-02 /
CHEB / 1.7515000e+01 5.4651000e-01 -3.2278000e-02 /
CHEB / -4.9884000e-01 4.3689000e-01 -1.4638000e-02 /
CHEB / -5.2987000e-01 2.9477000e-01 4.9318000e-03 /
CHEB / -4.2789000e-01 1.6037000e-01 1.8350000e-02 /

!PDepNetwork C4H8O-i1
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-i1          -38.26      82.01 24.81 30.17 35.04 39.27 46.13
      51.21 58.97 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
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!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H5OJ            27.09 76.26 18.34 21.54 24.52 27.2  31.62 34.9
      39.89 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H7             35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62
      50.57
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     iC4H7OJ(15)       -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33
      55.93 null
!     C4H7OJ(79)        13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41
      55.38 null
!     iC4H7OJ(17)       -1.97 78.93 25.6  30.87 35.26 38.89 44.56 48.86
      55.75  !MRH CBS-QB3 w/1DHR corrections
!Here are the path reactions and their high-P limit kinetics:
!     sC3H5+CH2OH=C4H8O-i1    1.4157154e+13      -0.15000
2.9166667e+02
!     C3H5OJ+CH3=C4H8O-i1     1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7+OH=C4H8O-i1       1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7OJ(15)+H=C4H8O-i1        5.0000000e+13      0.00000
0.0000000e+00
!     C4H7OJ(79)+H=C4H8O-i1         1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7OJ(17)+H=C4H8O-i1        5.0000000e+13      0.00000
0.0000000e+00

sC3H5+CH2OH(+m)=C4H8O-i1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_rad/H2/O          deltaHrxn(T=298K) = -
96.37005230756365 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2041000e+01 5.1505000e-01 -7.0952000e-02 /
CHEB / -1.3762000e+00 9.2197000e-01 -1.0930000e-01 /
CHEB / -1.0851000e+00 6.6779000e-01 -4.3717000e-02 /
CHEB / -7.5228000e-01 3.8776000e-01 1.1077000e-02 /
CHEB / -4.9017000e-01 1.7219000e-01 3.3549000e-02 /

sC3H5+CH2OH(+m)=iC4H7+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -14.22851959004161
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0009000e+01 -1.4344000e+00 -5.0852000e-02 /
CHEB / 1.5929000e+00 9.4207000e-01 -5.4958000e-02 /
CHEB / 2.3347000e-01 5.2979000e-01 2.5060000e-02 /
CHEB / -1.7242000e-01 1.5433000e-01 6.1807000e-02 /
CHEB / -1.6749000e-01 -4.5101000e-02 4.3677000e-02 /

sC3H5+CH2OH(+m)=iC4H7OJ(15)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -15.848848369867433
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 9.5422000e+00 -1.4430000e+00 -5.0118000e-02 /
CHEB / 2.2983000e+00 9.3251000e-01 -5.5379000e-02 /
CHEB / 4.1959000e-01 5.3385000e-01 2.2503000e-02 /
CHEB / -1.0063000e-01 1.6478000e-01 6.0294000e-02 /
CHEB / -1.4134000e-01 -3.7520000e-02 4.4817000e-02 /

sC3H5+CH2OH(+m)=iC4H7OJ(17)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -7.989766236049135
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6036000e+00 -1.4168000e+00 -5.2676000e-02 /
CHEB / 2.8319000e+00 9.6058000e-01 -5.4158000e-02 /
CHEB / 5.3930000e-01 5.1995000e-01 3.0587000e-02 /
CHEB / -7.9148000e-02 1.3294000e-01 6.4792000e-02 /
CHEB / -1.2496000e-01 -5.8982000e-02 4.1052000e-02 /

C3H5OJ+CH3(+m)=C4H8O-i1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_methyl      deltaHrxn(T=298K) = -
100.58941795118487 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1957000e+01 6.1156000e-01 -9.6137000e-02 /
CHEB / -1.5567000e+00 1.0658000e+00 -1.3742000e-01 /
CHEB / -1.1918000e+00 7.3409000e-01 -4.6021000e-02 /
CHEB / -7.9474000e-01 3.9913000e-01 1.8855000e-02 /
CHEB / -5.0499000e-01 1.6382000e-01 3.8017000e-02 /

C3H5OJ+CH3(+m)=sC3H5+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -4.219365643621215
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0116000e+01 -1.3383000e+00 -6.7144000e-02 /
CHEB / 2.2694000e+00 1.0189000e+00 -4.7609000e-02 /
CHEB / 3.4524000e-01 4.5664000e-01 5.8891000e-02 /
CHEB / -1.1644000e-01 5.0848000e-02 7.2447000e-02 /
CHEB / -1.1325000e-01 -9.2339000e-02 2.5239000e-02 /

C3H5OJ+CH3(+m)=iC4H7+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -18.447885233662827
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0378000e+01 -1.3986000e+00 -5.9255000e-02 /
CHEB / 1.2424000e+00 9.6960000e-01 -5.3480000e-02 /
CHEB / 1.5664000e-01 5.0439000e-01 3.8794000e-02 /
CHEB / -1.5026000e-01 1.1778000e-01 6.8209000e-02 /
CHEB / -1.4188000e-01 -6.2682000e-02 3.8599000e-02 /

C3H5OJ+CH3(+m)=iC4H7OJ(15)+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -20.06821401348865
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 9.8781000e+00 -1.4064000e+00 -5.8684000e-02 /
CHEB / 1.9775000e+00 9.6169000e-01 -5.4233000e-02 /
CHEB / 3.4225000e-01 5.0919000e-01 3.6409000e-02 /
CHEB / -8.1102000e-02 1.2729000e-01 6.7391000e-02 /
CHEB / -1.1577000e-01 -5.6782000e-02 4.0186000e-02 /

C3H5OJ+CH3(+m)=iC4H7OJ(17)+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -12.209131879670345
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0449000e+00 -1.3824000e+00 -6.0750000e-02 /
CHEB / 2.4110000e+00 9.8497000e-01 -5.2012000e-02 /
CHEB / 4.6754000e-01 4.9338000e-01 4.3882000e-02 /
CHEB / -5.1321000e-02 9.8530000e-02 6.9782000e-02 /
CHEB / -1.0006000e-01 -7.3376000e-02 3.5233000e-02 /

iC4H7+OH(+m)=C4H8O-i1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     O_pri_rad      deltaHrxn(T=298K) = -
82.14153271752204 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2304000e+01 3.1197000e-01 -2.9638000e-02 /
CHEB / -9.6693000e-01 5.8077000e-01 -4.9885000e-02 /
CHEB / -7.7833000e-01 4.6648000e-01 -2.6514000e-02 /
CHEB / -5.8608000e-01 3.1865000e-01 -2.7968000e-04 /
CHEB / -4.1841000e-01 1.7883000e-01 1.8416000e-02 /

iC4H7OJ(15)+H(+m)=C4H8O-i1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeO     H_rad       deltaHrxn(T=298K) = -
80.52120393769621 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3342000e+01 2.8652000e-01 -2.5580000e-02 /
CHEB / -8.4134000e-01 5.3555000e-01 -4.3328000e-02 /
CHEB / -7.0030000e-01 4.3546000e-01 -2.3554000e-02 /
CHEB / -5.3370000e-01 3.0388000e-01 -6.7118000e-04 /
CHEB / -3.8694000e-01 1.7645000e-01 1.6552000e-02 /

iC4H7OJ(15)+H(+m)=iC4H7+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = 1.6203287798258224
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8181000e+00 -1.5241000e+00 -3.7527000e-02 /
CHEB / 3.9168000e+00 8.3809000e-01 -5.1805000e-02 /
CHEB / 4.7442000e-01 5.5958000e-01 -1.4015000e-03 /
CHEB / -2.0050000e-01 2.5418000e-01 3.8071000e-02 /
CHEB / -2.2656000e-01 3.6327000e-02 4.4996000e-02 /

C4H7OJ(79)+H(+m)=C4H8O-i1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
104.04892333418195 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.1842000e+01 6.7100000e-01 -1.1338000e-01 /
CHEB / -1.6243000e+00 1.1462000e+00 -1.5301000e-01 /
CHEB / -1.2468000e+00 7.6639000e-01 -4.5568000e-02 /
CHEB / -8.3555000e-01 4.0239000e-01 2.3437000e-02 /
CHEB / -5.1841000e-01 1.5910000e-01 3.9641000e-02 /

C4H7OJ(79)+H(+m)=sC3H5+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -7.678871026618294
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0340000e+01 -1.3190000e+00 -7.2397000e-02 /
CHEB / 2.0165000e+00 1.0257000e+00 -4.4080000e-02 /
CHEB / 3.2618000e-01 4.3920000e-01 6.5728000e-02 /
CHEB / -1.1894000e-01 3.6496000e-02 7.2338000e-02 /
CHEB / -1.0974000e-01 -9.4839000e-02 2.1125000e-02 /

C4H7OJ(79)+H(+m)=C3H5OJ+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -3.4595053829970794
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2725000e+00 -1.2919000e+00 -7.7921000e-02 /
CHEB / 2.5237000e+00 1.0380000e+00 -3.9467000e-02 /
CHEB / 3.6951000e-01 4.1341000e-01 7.4626000e-02 /
CHEB / -1.0695000e-01 1.4082000e-02 7.1310000e-02 /
CHEB / -9.8845000e-02 -9.8972000e-02 1.4731000e-02 /

C4H7OJ(79)+H(+m)=iC4H7+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -21.907390616659907
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0479000e+01 -1.3763000e+00 -6.5411000e-02 /
CHEB / 1.1166000e+00 9.8175000e-01 -5.1096000e-02 /
CHEB / 1.2190000e-01 4.8702000e-01 4.7341000e-02 /
CHEB / -1.5915000e-01 9.8376000e-02 7.0717000e-02 /
CHEB / -1.3610000e-01 -6.9802000e-02 3.4860000e-02 /

C4H7OJ(79)+H(+m)=iC4H7OJ(15)+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -23.52771939648573
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9648000e+00 -1.3838000e+00 -6.4952000e-02 /
CHEB / 1.8635000e+00 9.7468000e-01 -5.2015000e-02 /
CHEB / 3.0786000e-01 4.9205000e-01 4.5127000e-02 /
CHEB / -9.0931000e-02 1.0724000e-01 7.0291000e-02 /
CHEB / -1.1000000e-01 -6.4741000e-02 3.6606000e-02 /

C4H7OJ(79)+H(+m)=iC4H7OJ(17)+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -15.668637262667424
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1766000e+00 -1.3610000e+00 -6.6682000e-02 /
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CHEB / 2.2577000e+00 9.9548000e-01 -4.9292000e-02 /
CHEB / 4.3334000e-01 4.7570000e-01 5.2044000e-02 /
CHEB / -5.8118000e-02 8.0482000e-02 7.1509000e-02 /
CHEB / -9.4470000e-02 -7.8936000e-02 3.1252000e-02 /

iC4H7OJ(17)+H(+m)=C4H8O-i1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
88.38028607151452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3397000e+01 3.6534000e-01 -3.8966000e-02 /
CHEB / -1.1554000e+00 6.7415000e-01 -6.4529000e-02 /
CHEB / -8.4424000e-01 5.2748000e-01 -3.2323000e-02 /
CHEB / -6.2025000e-01 3.4468000e-01 1.4318000e-03 /
CHEB / -4.3221000e-01 1.8060000e-01 2.2606000e-02 /

iC4H7OJ(17)+H(+m)=iC4H7+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -6.238753353992475
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0152000e+01 -1.4915000e+00 -4.1304000e-02 /
CHEB / 2.5316000e+00 8.8043000e-01 -5.3420000e-02 /
CHEB / 4.3229000e-01 5.5570000e-01 6.4864000e-03 /
CHEB / -1.8703000e-01 2.1938000e-01 4.7158000e-02 /
CHEB / -2.0397000e-01 1.4192000e-03 4.6729000e-02 /

iC4H7OJ(17)+H(+m)=iC4H7OJ(15)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i1)     deltaHrxn(T=298K) = -7.859082133818298
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7967000e+00 -1.5016000e+00 -4.0286000e-02 /
CHEB / 3.1185000e+00 8.6749000e-01 -5.3169000e-02 /
CHEB / 6.3514000e-01 5.5740000e-01 3.9733000e-03 /
CHEB / -1.0686000e-01 2.3060000e-01 4.4542000e-02 /
CHEB / -1.7852000e-01 1.2259000e-02 4.6564000e-02 /

!PDepNetwork C4H8O-i3 && C4H8O-i2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-i3          -51.2 79.65 23.57 29.46 34.96 39.45 46.7  51.93
      57.55 Estimated by Group Additivity
!     C4H8O-i2          -45.93      79.05 25.53 31.25 36.25 40.42 46.96
      51.79 59.42 Estimated by Group Additivity
!     CH3         35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03 16.21
      Primary Thermo Library: CFG (Species ID: CH3)
!     C3H5OJ(17)        19.42 73.31 19.06 22.62 25.73 28.35 32.45 35.48
      40.34 Estimated by Group Additivity
!     iC4H7OJ(15)       -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33
      55.93 Estimated by Group Additivity
!     H           52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96  4.96
      Primary Thermo Library: CFG (Species ID: H)
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!     HCC[CH3]2         55.3  72.75 21.39 25.9  29.94 33.42 39.09 43.4
      50.18 Estimated by Group Additivity
!     OH          8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23  7.72
      Primary Thermo Library: CFG (Species ID: OH)
!     iC4H7OJ(30)       -10.03      77.94 24.19 29.26 33.77 37.63 43.83
      48.46 55.63 Estimated by Group Additivity
!     C3H5OJ(12)        -4.96 71.27 18.06 21.58 24.93 27.85 32.53 36.02
      41.39 Primary Thermo Library: CFG (Species ID: CH3CHCHO)
!     iC4H7OJ(48)       -2.2  83.37 23.03 28.2  33.04 36.99 43.43 48.09
      53.71 Estimated by Group Additivity
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11 Primary Thermo Library: CFG (Species ID: ipropyl)
!     HCO         10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34 12.47
      Primary Thermo Library: CFG (Species ID: HCO)
!     iC4H7OJ(51)       -14.3 80.77 22.74 28.03 33.0  37.03 43.54 48.2
      52.91 Estimated by Group Additivity
!     C3H8              -24.27      66.07 17.76 22.39 26.7  30.47 36.6
      41.32 48.85 Primary Thermo Library: CFG (Species ID: C3H8)
!     CO          -26.44      47.14 6.95  6.99  7.09  7.24  7.57  7.87
      8.34  Primary Thermo Library: CFG (Species ID: CO)
!Here are the path reactions and their high-P limit kinetics:
!     C4H8O-i2=C4H8O-i3             8.590e+11    0.32        55900.00
!     CH3+C3H5OJ(17)=C4H8O-i2       1.000e+13    0.00        0.00
!     iC4H7OJ(15)+H=C4H8O-i2        5.000e+13    0.00        0.00
!     HCC[CH3]2+OH=C4H8O-i2         1.000e+13    0.00        0.00
!     iC4H7OJ(30)+H=C4H8O-i2        1.000e+13    0.00        0.00
!     CH3+C3H5OJ(12)=C4H8O-i3       6.800e+14    -0.68       0.00
!     iC4H7OJ(48)+H=C4H8O-i3        1.000e+14    0.00        0.00
!     C3H7-2+HCO=C4H8O-i3     1.000e+13    0.00        0.00
!     iC4H7OJ(30)+H=C4H8O-i3        5.000e+13    0.00        0.00
!     iC4H7OJ(51)+H=C4H8O-i3        1.000e+13    0.00        0.00
!     C3H8+CO=C4H8O-i3        7.660e+05    2.07        82200.00

C4H8O-i2(+m)=C4H8O-i3(+m)                        1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
ReactionLibrary: Tautomerization    deltaHrxn(T=298K) = -
5.269267092314351 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.0800000e+01 2.3477000e-01 -3.8710000e-02 -9.0653000e-04 /
CHEB / 1.6965000e+01 4.4254000e-01 -6.9397000e-02 -3.0007000e-03 /
CHEB / -3.5662000e-01 3.7009000e-01 -4.8709000e-02 -5.7291000e-03 /
CHEB / -2.9460000e-01 2.7362000e-01 -2.3512000e-02 -8.1536000e-03 /

CH3+C3H5OJ(17)(+m)=C4H8O-i3(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -105.85868501778268 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0894000e+01 -4.3500000e-01 -3.8171000e-01 6.0796000e-02 /
CHEB / -2.6767000e-01 1.9887000e+00 -2.5300000e-01 -3.8916000e-02 /
CHEB / -5.7697000e-01 9.5533000e-01 1.0005000e-02 -5.6087000e-02 /
CHEB / -3.9985000e-01 3.3862000e-01 7.5859000e-02 -2.9522000e-02 /

CH3+C3H5OJ(17)(+m)=C4H8O-i2(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
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R_Recombination estimate: (Average:) [ C_methyl , Cd_rad/NonDe ]
      deltaHrxn(T=298K) = -100.58941792546833 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2290000e+01 9.7608000e-01 -2.6091000e-01 4.0102000e-02 /
CHEB / -1.3812000e+00 1.4132000e+00 -2.4447000e-01 -2.6219000e-02 /
CHEB / -8.3736000e-01 7.5969000e-01 -8.4942000e-03 -6.4589000e-02 /
CHEB / -4.4285000e-01 3.1963000e-01 7.5241000e-02 -3.9493000e-02 /

iC4H7OJ(15)+H(+m)=C4H8O-i3(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -93.45976498191807 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1388000e+01 -1.0749000e+00 -1.7061000e-01 1.1251000e-02 /
CHEB / 7.0364000e-01 1.5166000e+00 -2.1907000e-01 -1.0227000e-02 /
CHEB / -2.4075000e-01 8.8894000e-01 -4.0703000e-02 -3.6000000e-02 /
CHEB / -3.3992000e-01 3.7937000e-01 4.6954000e-02 -2.7323000e-02 /

iC4H7OJ(15)+H(+m)=C4H8O-i2(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/Cd , H_rad ]
      deltaHrxn(T=298K) = -88.19049788960372 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3363000e+01 5.2156000e-01 -1.0599000e-01 1.9050000e-03 /
CHEB / -9.1094000e-01 8.8864000e-01 -1.4543000e-01 -1.5891000e-02 /
CHEB / -6.0531000e-01 5.9059000e-01 -4.1582000e-02 -3.3000000e-02 /
CHEB / -3.6969000e-01 3.1524000e-01 2.6060000e-02 -2.9357000e-02 /

iC4H7OJ(15)+H(+m)=CH3+C3H5OJ(17)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 12.398920035864613 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.4501000e+00 -1.3103000e+00 -1.2550000e-01 1.4902000e-02 /
CHEB / 6.2590000e+00 9.4362000e-01 -6.4868000e-02 -2.7934000e-02 /
CHEB / 4.4860000e-01 3.7568000e-01 8.1438000e-02 -3.1753000e-02 /
CHEB / -3.0564000e-03 5.5416000e-02 8.4232000e-02 2.7624000e-03 /

HCC[CH3]2+OH(+m)=C4H8O-i3(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -115.177750672624 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0609000e+01 3.2349000e-01 -6.2739000e-01 1.0470000e-01 /
CHEB / -8.1988000e-01 2.2851000e+00 -2.6963000e-01 -4.3684000e-02 /
CHEB / -7.7142000e-01 9.7925000e-01 4.9286000e-02 -7.9582000e-02 /
CHEB / -4.4636000e-01 3.1023000e-01 9.8072000e-02 -3.6607000e-02 /

HCC[CH3]2+OH(+m)=C4H8O-i2(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ Cd_pri_rad , O_pri_rad ]
      deltaHrxn(T=298K) = -109.90848358030965 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1805000e+01 1.5349000e+00 -4.8471000e-01 1.0634000e-01 /
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CHEB / -1.7597000e+00 1.8618000e+00 -3.1113000e-01 -5.3965000e-02 /
CHEB / -9.9186000e-01 8.4087000e-01 4.6675000e-02 -9.7096000e-02 /
CHEB / -4.9489000e-01 2.9640000e-01 1.1529000e-01 -4.1973000e-02 /

HCC[CH3]2+OH(+m)=CH3+C3H5OJ(17)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -9.319065654841324 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7352000e+00 -1.1787000e+00 -1.5589000e-01 2.2381000e-02 /
CHEB / 2.4600000e+00 9.5187000e-01 -1.3890000e-02 -4.4825000e-02 /
CHEB / 5.3128000e-01 2.9403000e-01 1.1247000e-01 -2.1540000e-02 /
CHEB / 1.2972000e-02 8.2403000e-03 6.9432000e-02 1.8915000e-02 /

HCC[CH3]2+OH(+m)=iC4H7OJ(15)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -21.717985690705937 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.3268000e+00 -1.2090000e+00 -1.5814000e-01 2.4399000e-02 /
CHEB / 2.1683000e+00 9.2912000e-01 -2.2285000e-02 -4.5537000e-02 /
CHEB / 5.1737000e-01 3.1902000e-01 1.0447000e-01 -2.6042000e-02 /
CHEB / 5.3232000e-02 3.0584000e-02 7.4430000e-02 1.4701000e-02 /

iC4H7OJ(30)+H(+m)=C4H8O-i3(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/Cs2 , H_rad ]
      deltaHrxn(T=298K) = -93.25983539490554 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3379000e+01 4.0619000e-01 -7.1955000e-02 6.5672000e-03 /
CHEB / -8.8602000e-01 6.8032000e-01 -9.6194000e-02 1.0436000e-04 /
CHEB / -5.8169000e-01 4.3023000e-01 -2.8286000e-02 -9.2835000e-03 /
CHEB / -3.4753000e-01 2.1331000e-01 7.6090000e-03 -6.6160000e-03 /

iC4H7OJ(30)+H(+m)=C4H8O-i2(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ O_rad/OneDe , H_rad ]
      deltaHrxn(T=298K) = -87.99056830259119 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2864000e+01 3.6134000e-01 -6.5941000e-02 -9.7587000e-04 /
CHEB / -7.5108000e-01 6.8432000e-01 -1.2166000e-01 -2.0031000e-03 /
CHEB / -5.0694000e-01 5.2946000e-01 -6.5496000e-02 -1.4134000e-02 /
CHEB / -3.4136000e-01 3.1948000e-01 7.6437000e-04 -2.2210000e-02 /

iC4H7OJ(30)+H(+m)=CH3+C3H5OJ(17)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 12.59884962287714 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.8410000e+00 -1.3357000e+00 -1.2106000e-01 1.5526000e-02 /
CHEB / 6.2305000e+00 9.5156000e-01 -7.3754000e-02 -2.7334000e-02 /
CHEB / 4.4885000e-01 3.9031000e-01 8.0143000e-02 -3.4151000e-02 /
CHEB / -9.2825000e-03 5.9462000e-02 8.7411000e-02 2.0645000e-03 /
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iC4H7OJ(30)+H(+m)=iC4H7OJ(15)+H(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 0.1999295870125266 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.8726000e+00 -1.4478000e+00 -8.6720000e-02 3.0317000e-03 /
CHEB / 4.3755000e+00 9.0927000e-01 -1.0336000e-01 -1.0442000e-02 /
CHEB / 7.3090000e-01 4.6878000e-01 3.1767000e-02 -2.9907000e-02 /
CHEB / 2.0689000e-02 1.1683000e-01 8.4645000e-02 -1.3315000e-02 /

HCC[CH3]2+OH(+m)=iC4H7OJ(30)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -21.917915277718457 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.8470000e+00 -1.2211000e+00 -1.5930000e-01 2.5782000e-02 /
CHEB / 1.9475000e+00 9.3292000e-01 -2.4650000e-02 -4.7112000e-02 /
CHEB / 4.6715000e-01 3.2606000e-01 1.0569000e-01 -2.7147000e-02 /
CHEB / 3.7451000e-02 3.2563000e-02 7.6048000e-02 1.4998000e-02 /

CH3+C3H5OJ(12)(+m)=C4H8O-i3(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ C_methyl , C_rad/H/OneDeC ]
      deltaHrxn(T=298K) = -81.48126765920613 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2713000e+01 2.5624000e-01 -3.5696000e-02 7.8813000e-04 /
CHEB / -8.4873000e-01 4.6011000e-01 -5.6312000e-02 -1.1273000e-03 /
CHEB / -4.9314000e-01 3.3480000e-01 -2.4682000e-02 -4.9995000e-03 /
CHEB / -2.9760000e-01 1.9734000e-01 1.5653000e-03 -5.1823000e-03 /

CH3+C3H5OJ(12)(+m)=C4H8O-i2(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -76.21200056689177 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.6907000e+00 -1.2953000e+00 -1.0635000e-01 2.7541000e-03 /
CHEB / 1.3111000e+00 1.2220000e+00 -1.5649000e-01 -5.6007000e-03 /
CHEB / -7.8748000e-02 7.9943000e-01 -4.7107000e-02 -2.0555000e-02 /
CHEB / -3.3096000e-01 3.8879000e-01 2.8297000e-02 -2.0369000e-02 /

CH3+C3H5OJ(17)(+m)=CH3+C3H5OJ(12)(+m)          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -24.377417358576558 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0586000e+01 -2.3193000e+00 -2.9102000e-01 3.4342000e-02 /
CHEB / 1.7193000e+00 1.8031000e+00 -2.5784000e-03 -7.0600000e-02 /
CHEB / 2.0683000e-01 5.6789000e-01 1.5178000e-01 -2.9295000e-02 /
CHEB / -1.0434000e-01 3.1893000e-02 9.9386000e-02 8.7578000e-03 /

iC4H7OJ(15)+H(+m)=CH3+C3H5OJ(12)(+m)           1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -11.978497322711945 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7979000e+00 -2.7291000e+00 -1.7562000e-01 1.0028000e-02 /
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CHEB / 3.2499000e+00 1.8589000e+00 -1.3637000e-01 -2.8275000e-02 /
CHEB / 3.6515000e-01 7.7096000e-01 8.6310000e-02 -3.8275000e-02 /
CHEB / -1.7562000e-01 1.2795000e-01 1.0831000e-01 -6.9826000e-03 /

HCC[CH3]2+OH(+m)=CH3+C3H5OJ(12)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -33.69648301341788 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1106000e+01 -1.8881000e+00 -3.8339000e-01 2.8438000e-02 /
CHEB / 1.1428000e+00 1.5480000e+00 1.3892000e-01 -7.6850000e-02 /
CHEB / 1.1791000e-01 4.2944000e-01 1.6591000e-01 -1.6143000e-02 /
CHEB / -9.0168000e-02 1.6014000e-03 7.5917000e-02 2.1024000e-02 /

iC4H7OJ(30)+H(+m)=CH3+C3H5OJ(12)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -11.778567735699419 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1682000e+01 -1.3685000e+00 -7.5882000e-02 4.8656000e-03 /
CHEB / 1.5931000e+00 9.4617000e-01 -5.6963000e-02 -1.0980000e-02 /
CHEB / 2.2439000e-01 4.1244000e-01 4.5130000e-02 -1.4522000e-02 /
CHEB / -1.0451000e-01 6.8745000e-02 5.4316000e-02 4.8893000e-04 /

iC4H7OJ(48)+H(+m)=C4H8O-i3(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination exact:  [ C_rad/H2/Cs , H_rad ] deltaHrxn(T=298K) = -
101.08917482055664 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3333000e+01 7.0103000e-01 -1.6202000e-01 3.2622000e-02 /
CHEB / -1.1570000e+00 9.1211000e-01 -9.3330000e-02 -1.7761000e-02 /
CHEB / -7.2403000e-01 4.6315000e-01 9.7132000e-03 -1.4590000e-02 /
CHEB / -3.9530000e-01 1.8460000e-01 2.4942000e-02 2.8671000e-03 /

iC4H7OJ(48)+H(+m)=C4H8O-i2(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -95.81990772824228 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1491000e+01 -7.0950000e-01 -2.7213000e-01 4.1125000e-02 /
CHEB / 1.1279000e-01 1.7914000e+00 -2.0245000e-01 -3.0940000e-02 /
CHEB / -5.1624000e-01 8.8922000e-01 2.0134000e-02 -4.4594000e-02 /
CHEB / -4.1427000e-01 3.2151000e-01 7.0989000e-02 -1.9070000e-02 /

iC4H7OJ(48)+H(+m)=CH3+C3H5OJ(17)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 4.769510197226047 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.1871000e+00 -2.1250000e+00 -3.0414000e-01 2.6045000e-02 /
CHEB / 5.2425000e+00 1.7771000e+00 5.4126000e-02 -6.7838000e-02 /
CHEB / 4.9543000e-01 4.3926000e-01 1.5968000e-01 -1.2349000e-02 /
CHEB / -6.1145000e-02 -1.8236000e-02 7.5681000e-02 1.5405000e-02 /
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iC4H7OJ(48)+H(+m)=iC4H7OJ(15)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -7.629409838638566 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.6382000e+00 -2.4151000e+00 -2.4673000e-01 2.4556000e-02 /
CHEB / 4.1907000e+00 1.8757000e+00 -4.3650000e-02 -5.5588000e-02 /
CHEB / 6.2617000e-01 5.7638000e-01 1.4484000e-01 -2.7683000e-02 /
CHEB / -4.2276000e-02 2.4249000e-02 9.4969000e-02 8.6098000e-03 /

HCC[CH3]2+OH(+m)=iC4H7OJ(48)+H(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -14.088575852067372 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.2811000e+00 -1.7982000e+00 -3.5658000e-01 1.4607000e-02 /
CHEB / 2.9511000e+00 1.5422000e+00 1.5257000e-01 -5.9769000e-02 /
CHEB / 5.2525000e-01 3.5907000e-01 1.4951000e-01 -3.4347000e-03 /
CHEB / 1.5669000e-03 -2.7974000e-02 5.8572000e-02 1.9216000e-02 /

iC4H7OJ(30)+H(+m)=iC4H7OJ(48)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 7.829339425651092 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.1642000e+00 -1.1417000e+00 -1.2891000e-01 1.6147000e-02 /
CHEB / 4.9999000e+00 9.6338000e-01 1.0359000e-02 -3.3035000e-02 /
CHEB / 4.6420000e-01 2.6468000e-01 8.7806000e-02 -5.6265000e-03 /
CHEB / 8.3648000e-03 -1.9268000e-02 3.9528000e-02 1.3148000e-02 /

iC4H7OJ(48)+H(+m)=CH3+C3H5OJ(12)(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -19.60790716135051 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2597000e+01 -1.1930000e+00 -1.2457000e-01 1.7847000e-02 /
CHEB / 9.0605000e-01 9.6177000e-01 -3.9566000e-03 -3.2208000e-02 /
CHEB / 1.2870000e-01 3.1100000e-01 8.5376000e-02 -1.1361000e-02 /
CHEB / -6.9826000e-02 2.9089000e-03 5.0534000e-02 1.1886000e-02 /

C3H7-2+HCO(+m)=C4H8O-i3(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3) High-P Limit: R_Recombination estimate:
(Average:) [ C_rad/H/NonDeC , CO_pri_rad ]      deltaHrxn(T=298K) = -
87.28108989664476 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2671000e+01 3.4022000e-01 -5.2370000e-02 3.3659000e-03 /
CHEB / -7.3375000e-01 5.8861000e-01 -7.4591000e-02 -3.3622000e-04 /
CHEB / -5.2706000e-01 3.9237000e-01 -2.2491000e-02 -7.4182000e-03 /
CHEB / -3.3137000e-01 2.0453000e-01 1.0241000e-02 -5.7902000e-03 /

C3H7-2+HCO(+m)=C4H8O-i2(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
82.01182280433041 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0106000e+01 -1.1713000e+00 -1.3312000e-01 6.9679000e-03 /
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CHEB / 1.0708000e+00 1.3920000e+00 -1.7899000e-01 -6.7370000e-03 /
CHEB / -1.9350000e-01 8.4795000e-01 -3.4904000e-02 -2.6971000e-02 /
CHEB / -3.5824000e-01 3.7448000e-01 4.3734000e-02 -2.1992000e-02 /

CH3+C3H5OJ(17)(+m)=C3H7-2+HCO(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
18.577595121137925 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0616000e+01 -2.2722000e+00 -2.9225000e-01 3.2223000e-02 /
CHEB / 1.9979000e+00 1.8058000e+00 1.1686000e-02 -7.0085000e-02 /
CHEB / 2.6416000e-01 5.3300000e-01 1.5503000e-01 -2.4090000e-02 /
CHEB / -9.6239000e-02 1.3443000e-02 9.2762000e-02 1.1509000e-02 /

iC4H7OJ(15)+H(+m)=C3H7-2+HCO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
6.178675085273314 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.5870000e+00 -2.6576000e+00 -1.8739000e-01 1.2326000e-02 /
CHEB / 3.7493000e+00 1.8916000e+00 -1.2149000e-01 -3.2710000e-02 /
CHEB / 3.7923000e-01 7.2196000e-01 1.0589000e-01 -3.7231000e-02 /
CHEB / -1.6660000e-01 9.0192000e-02 1.0847000e-01 -2.3448000e-03 /

HCC[CH3]2+OH(+m)=C3H7-2+HCO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
27.89666077597925 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1258000e+01 -1.8667000e+00 -3.7459000e-01 2.4281000e-02 /
CHEB / 1.3337000e+00 1.5476000e+00 1.4344000e-01 -7.1677000e-02 /
CHEB / 1.7352000e-01 4.1134000e-01 1.6004000e-01 -1.1465000e-02 /
CHEB / -8.0344000e-02 -8.0232000e-03 6.9951000e-02 2.0673000e-02 /

iC4H7OJ(30)+H(+m)=C3H7-2+HCO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
5.978745498260787 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1400000e+01 -1.3209000e+00 -8.3042000e-02 6.1834000e-03 /
CHEB / 2.1383000e+00 9.7502000e-01 -4.8798000e-02 -1.3691000e-02 /
CHEB / 2.7321000e-01 3.8003000e-01 5.8940000e-02 -1.4250000e-02 /
CHEB / -9.6256000e-02 3.7241000e-02 5.4919000e-02 3.7317000e-03 /

C3H7-2+HCO(+m)=CH3+C3H5OJ(12)(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
5.799822237438634 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0401000e+01 -1.4032000e+00 -6.6644000e-02 2.7085000e-03 /
CHEB / 2.1063000e+00 9.3264000e-01 -6.1138000e-02 -8.1819000e-03 /
CHEB / 2.6239000e-01 4.4085000e-01 3.6140000e-02 -1.3701000e-02 /
CHEB / -1.2943000e-01 8.9818000e-02 5.5779000e-02 -9.7295000e-04 /

iC4H7OJ(48)+H(+m)=C3H7-2+HCO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
13.80808492391188 kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2515000e+01 -1.1548000e+00 -1.2803000e-01 1.7296000e-02 /
CHEB / 1.2620000e+00 9.7392000e-01 5.7823000e-03 -3.3592000e-02 /
CHEB / 2.0791000e-01 2.8108000e-01 9.1753000e-02 -8.5061000e-03 /
CHEB / -5.5219000e-02 -1.8132000e-02 4.6196000e-02 1.4291000e-02 /

iC4H7OJ(51)+H(+m)=C4H8O-i3(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3) High-P Limit:
R_Recombination estimate: (Average:) [ CO_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -88.99041148107514 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2645000e+01 3.4815000e-01 -5.4124000e-02 3.6894000e-03 /
CHEB / -7.3328000e-01 5.9991000e-01 -7.6203000e-02 -2.9922000e-04 /
CHEB / -5.3583000e-01 3.9661000e-01 -2.2043000e-02 -7.6838000e-03 /
CHEB / -3.2878000e-01 2.0457000e-01 1.1027000e-02 -5.7821000e-03 /

iC4H7OJ(51)+H(+m)=C4H8O-i2(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -83.72114438876079 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0112000e+01 -1.1599000e+00 -1.3581000e-01 7.4633000e-03 /
CHEB / 1.0468000e+00 1.4064000e+00 -1.8085000e-01 -6.9185000e-03 /
CHEB / -2.0797000e-01 8.5119000e-01 -3.3578000e-02 -2.7584000e-02 /
CHEB / -3.5520000e-01 3.7293000e-01 4.4981000e-02 -2.2060000e-02 /

iC4H7OJ(51)+H(+m)=CH3+C3H5OJ(17)(+m)           1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= 16.868273536707548 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 2.5472000e+00 -2.2681000e+00 -2.9243000e-01 3.2038000e-02 /
CHEB / 7.9257000e+00 1.8058000e+00 1.2897000e-02 -7.0036000e-02 /
CHEB / 3.5720000e-01 5.3001000e-01 1.5528000e-01 -2.3675000e-02 /
CHEB / -8.3328000e-02 1.2039000e-02 9.2210000e-02 1.1703000e-02 /

iC4H7OJ(15)+H(+m)=iC4H7OJ(51)+H(+m)            1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -4.469353500842935 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.1046000e+00 -2.6513000e+00 -1.8860000e-01 1.2575000e-02 /
CHEB / 4.6149000e+00 1.8936000e+00 -1.2000000e-01 -3.3173000e-02 /
CHEB / 5.6044000e-01 7.1748000e-01 1.0750000e-01 -3.7106000e-02 /
CHEB / -1.1232000e-01 8.7285000e-02 1.0833000e-01 -1.9518000e-03 /

HCC[CH3]2+OH(+m)=iC4H7OJ(51)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -26.187339191548865 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.8065000e+00 -1.8648000e+00 -3.7390000e-01 2.3945000e-02 /
CHEB / 2.1711000e+00 1.5476000e+00 1.4378000e-01 -7.1262000e-02 /
CHEB / 3.5922000e-01 4.0977000e-01 1.5961000e-01 -1.1124000e-02 /
CHEB / -2.6282000e-02 -8.7942000e-03 6.9505000e-02 2.0634000e-02 /
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iC4H7OJ(30)+H(+m)=iC4H7OJ(51)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -4.269423913830401 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.9105000e+00 -1.3166000e+00 -8.3821000e-02 6.3405000e-03 /
CHEB / 3.0095000e+00 9.7694000e-01 -4.7919000e-02 -1.3994000e-02 /
CHEB / 4.5679000e-01 3.7684000e-01 6.0136000e-02 -1.4197000e-02 /
CHEB / -4.2113000e-02 3.4732000e-02 5.4814000e-02 4.0326000e-03 /

iC4H7OJ(51)+H(+m)=CH3+C3H5OJ(12)(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -7.509143821869011 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0442000e+01 -1.3982000e+00 -6.7597000e-02 2.9213000e-03 /
CHEB / 2.0614000e+00 9.3636000e-01 -6.0619000e-02 -8.4663000e-03 /
CHEB / 2.5628000e-01 4.3790000e-01 3.7801000e-02 -1.3872000e-02 /
CHEB / -1.2170000e-01 8.6360000e-02 5.6211000e-02 -6.8387000e-04 /

iC4H7OJ(48)+H(+m)=iC4H7OJ(51)+H(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K)
= -12.0987633394815 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.0429000e+00 -1.1513000e+00 -1.2844000e-01 1.7262000e-02 /
CHEB / 2.1152000e+00 9.7458000e-01 6.7139000e-03 -3.3734000e-02 /
CHEB / 3.9515000e-01 2.7831000e-01 9.2273000e-02 -8.2423000e-03 /
CHEB / -8.6902000e-04 -1.9776000e-02 4.5753000e-02 1.4487000e-02 /

iC4H7OJ(51)+H(+m)=C3H7-2+HCO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
1.7093215844303788 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0039000e+01 -1.3468000e+00 -7.5664000e-02 4.4679000e-03 /
CHEB / 2.7367000e+00 9.7383000e-01 -5.4128000e-02 -1.1149000e-02 /
CHEB / 2.7249000e-01 4.0568000e-01 5.3969000e-02 -1.4653000e-02 /
CHEB / -1.1248000e-01 4.9812000e-02 5.9126000e-02 2.6320000e-03 /

C4H8O-i3(+m)=C3H8+CO(+m)                  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) =
0.4898339121092441 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.0639000e+01 2.7297000e-01 -3.8752000e-02 1.1891000e-03 /
CHEB / 2.5290000e+01 4.8685000e-01 -6.0049000e-02 -9.4327000e-04 /
CHEB / -4.3165000e-01 3.4818000e-01 -2.4631000e-02 -5.4176000e-03 /
CHEB / -3.0254000e-01 2.0000000e-01 3.2749000e-03 -5.3925000e-03 /

C4H8O-i2(+m)=C3H8+CO(+m)                  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
4.779433180205107 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.1298000e+01 -1.2700000e+00 -1.1142000e-01 3.4472000e-03 /
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CHEB / 2.5609000e+01 1.2583000e+00 -1.6132000e-01 -5.7382000e-03 /
CHEB / -7.3830000e-02 8.1139000e-01 -4.5003000e-02 -2.1797000e-02 /
CHEB / -3.3918000e-01 3.8646000e-01 3.1665000e-02 -2.0824000e-02 /

CH3+C3H5OJ(17)(+m)=C3H8+CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
105.36885110567344 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.0675000e+00 -2.3094000e+00 -2.9115000e-01 3.3897000e-02 /
CHEB / 2.5940000e+00 1.8041000e+00 5.0878000e-04 -7.0496000e-02 /
CHEB / 4.0035000e-01 5.6045000e-01 1.5252000e-01 -2.8124000e-02 /
CHEB / -4.9195000e-02 2.7637000e-02 9.7939000e-02 9.4286000e-03 /

iC4H7OJ(15)+H(+m)=C3H8+CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
92.96993106980884 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.2289000e+00 -2.7142000e+00 -1.7779000e-01 1.0433000e-02 /
CHEB / 4.1692000e+00 1.8671000e+00 -1.3353000e-01 -2.9089000e-02 /
CHEB / 5.5072000e-01 7.6108000e-01 9.0561000e-02 -3.8100000e-02 /
CHEB / -1.2082000e-01 1.1934000e-01 1.0862000e-01 -5.9885000e-03 /

HCC[CH3]2+OH(+m)=C3H8+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
114.68791676051477 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.6142000e+00 -1.8837000e+00 -3.8139000e-01 2.7513000e-02 /
CHEB / 1.9997000e+00 1.5478000e+00 1.3999000e-01 -7.5689000e-02 /
CHEB / 3.1068000e-01 4.2562000e-01 1.6452000e-01 -1.5023000e-02 /
CHEB / -3.4709000e-02 -5.4528000e-04 7.4510000e-02 2.0973000e-02 /

iC4H7OJ(30)+H(+m)=C3H8+CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
92.7700014827963 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.0995000e+00 -1.3587000e+00 -7.7150000e-02 5.0793000e-03 /
CHEB / 2.5194000e+00 9.5320000e-01 -5.5472000e-02 -1.1456000e-02 /
CHEB / 4.1825000e-01 4.0631000e-01 4.8030000e-02 -1.4502000e-02 /
CHEB / -4.9610000e-02 6.1762000e-02 5.4712000e-02 1.1383000e-03 /

CH3+C3H5OJ(12)(+m)=C3H8+CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
80.99143374709688 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.8171000e+00 -1.4475000e+00 -5.9437000e-02 1.2975000e-03 /
CHEB / 3.7405000e+00 8.9332000e-01 -6.4149000e-02 -6.3094000e-03 /
CHEB / 4.1504000e-01 4.6239000e-01 2.1873000e-02 -1.2072000e-02 /
CHEB / -1.0357000e-01 1.2202000e-01 5.0328000e-02 -3.1055000e-03 /

iC4H7OJ(48)+H(+m)=C3H8+CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
100.5993409084474 kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0056000e+01 -1.1852000e+00 -1.2513000e-01 1.7708000e-02 /
CHEB / 1.7953000e+00 9.6497000e-01 -2.0221000e-03 -3.2464000e-02 /
CHEB / 3.2724000e-01 3.0500000e-01 8.6773000e-02 -1.0781000e-02 /
CHEB / -1.3101000e-02 -1.8324000e-03 4.9733000e-02 1.2415000e-02 /

C3H7-2+HCO(+m)=C3H8+CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O-i3)     deltaHrxn(T=298K) = -86.79125598453551
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.7899000e+00 -1.3926000e+00 -6.8079000e-02 2.9489000e-03 /
CHEB / 3.0623000e+00 9.4186000e-01 -6.0101000e-02 -8.6208000e-03 /
CHEB / 4.4970000e-01 4.3514000e-01 3.9485000e-02 -1.3915000e-02 /
CHEB / -7.5068000e-02 8.1765000e-02 5.6782000e-02 -3.5758000e-04 /

iC4H7OJ(51)+H(+m)=C3H8+CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O-i3)      deltaHrxn(T=298K) = -
88.5005775689659 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.8347000e+00 -1.3876000e+00 -6.9021000e-02 3.1599000e-03 /
CHEB / 3.0137000e+00 9.4535000e-01 -5.9530000e-02 -8.9137000e-03 /
CHEB / 4.4455000e-01 4.3208000e-01 4.1114000e-02 -1.4063000e-02 /
CHEB / -6.7286000e-02 7.8386000e-02 5.7139000e-02 -5.6613000e-05 /

!PDepNetwork C4H9O-1 + C4H9O-2 + C4H9O-3 + C4H9O-4 + C4H9O-5
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9O-1           -16.27      88.99 26.95 32.82 38.15 42.65 49.68
      54.93 63.28  !MRH
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H9O-5           -13.43      82.96 26.61 32.68 38.16 42.84 50.26
      55.81 64.46  !MRH
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C4H8O-enol3             -35.91      84.25 23.67 29.6  34.76 39.15
      46.07 51.14 56.94 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
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!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     C4H8O-enol2             -37.68      83.04 23.93 29.26 34.16 38.51
      45.56 50.76 58.66 null
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H8O-enol        -42.24      81.3  24.52 30.69 35.99 40.36 47.01
      51.87 59.46 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9-1            20.65 78.53 23.01 28.55 33.6  37.94 44.89 50.17
      58.56
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+C2H5O-1=C4H9O-1    1.9900000e+03      2.44000
5.3700000e+03
!     C4H8O-enol3+H=C4H9O-1         1.1800000e+13      0.00000
3.8000000e+03
!     C4H7-14+H2O=C4H9O-1           2.2700000e+02      2.74000
5.6900000e+04
!     C4H9O-1=C4H9O-3               2.3600000e+10      0.82000
3.5100000e+04
!     CH3+C3H6O-enol2=C4H9O-3       3.1000000e+12      0.00000
8.5000000e+03
!     C4H8O-enol2+H=C4H9O-3         1.0000000e+13      0.00000
2.9000000e+03
!     C4H8-1+OH=C4H9O-3       2.7100000e+12      0.00000
0.0000000e+00
!     C4H8O-enol+H=C4H9O-3          1.0000000e+13      0.00000
2.9000000e+03
!     C4H9O-5=C4H9O-3               9.7200000e+09      1.17000
3.9660000e+04
!     C3H7-1+CH2O=C4H9O-5     7.9400000e+10      0.00000
6.7000000e+03
!     nC4H8O+H=C4H9O-5        1.0000000e+11      0.00000
1.1900000e+04
!     C4H9O-5=C4H9O-4               8.1282219e+08      1.13906
3.4790987e+04
!     nC4H8O+H=C4H9O-4        2.500e+11    0.18        2985.00
!     C2H5+C2H4O=C4H9O-4      1.9900000e+03      2.44000
5.3700000e+03
!     C4H8O-enol+H=C4H9O-4          1.0000000e+13      0.00000
2.9000000e+03
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!     C4H9O-2=C4H9O-4               9.7992653e+09      0.74500
3.2600000e+04
!     C4H8O-enol3+H=C4H9O-2         2.0100000e+13      0.00000
2.1000000e+03
!     C3H6+CH2OH=C4H9O-2      2.4100000e+10      0.00000
6.9600000e+03
!     C4H8O-enol2+H=C4H9O-2         1.0000000e+13      0.00000
2.9000000e+03
!     C4H9O-1=C4H9O-2               3.8760000e+10      0.89000
3.5800000e+04
!     C4H9O-3=C4H9O-2               1.3520000e+10      0.88000
3.8000000e+04
!     C4H9O-5=C4H9O-2               4.0000000e+11      0.00000
2.6850000e+04
!     C4H9O-3=C4H9O-4               1.3103945e+11      0.63800
3.9880000e+04
!     C4H9O-1=C4H9O-4               1.2880000e+10      0.13000
2.0700000e+04
!     C4H9O-5=C4H9O-1               1.1250000e+11      0.00000
2.4400000e+04
!     C4H9-1+O=C4H9O-5        1.0000000e+13      0.00000
0.0000000e+00

C4H9O-1(+m)=C4H9O-3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration exact:  Others-R3H_SS
C_rad_out_2H     Cs_H_out_H/NonDeC        deltaHrxn(T=298K) = -
2.230002825941977 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1328000e+00 1.4232000e+00 -3.2494000e-01 /
CHEB / 6.4647000e+00 1.3579000e+00 -2.8319000e-02 /
CHEB / -3.8145000e+00 2.8123000e-01 9.5623000e-02 /
CHEB / -2.2150000e+00 -2.6461000e-01 6.1258000e-02 /
CHEB / -1.0282000e+00 -3.3193000e-01 -1.2487000e-02 /

C4H9O-1(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
R4H_SSS     C_rad_out_2H     Cs_H_out_H/NonDeO        deltaHrxn(T=298K)
= -6.859238675343352 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0039000e-01 4.9027000e-01 -3.5277000e-02 /
CHEB / 2.3296000e+00 7.4492000e-01 -2.8788000e-02 /
CHEB / -3.5389000e+00 2.3753000e-01 3.9843000e-02 /
CHEB / -2.1789000e+00 -1.7270000e-01 5.3466000e-02 /
CHEB / -1.0329000e+00 -2.9392000e-01 6.2342000e-03 /

C4H9O-1(+m)=C4H9O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/(NonDeC/Cs)
      deltaHrxn(T=298K) = -3.42975638096393 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7521000e+00 9.6025000e-01 -2.4496000e-02 /
CHEB / 6.9781000e+00 1.7144000e+00 -1.7125000e-01 /
CHEB / -3.5694000e+00 1.7498000e-01 1.7364000e-01 /
CHEB / -2.1994000e+00 -2.5279000e-01 9.7946000e-02 /
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CHEB / -1.0696000e+00 -3.6336000e-01 -5.5506000e-03 /

C4H9O-3(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_H/NonDeC     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -4.6292358494013754 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9606000e+00 1.2623000e+00 -1.3268000e-01 /
CHEB / 7.6193000e+00 1.4727000e+00 -4.2712000e-02 /
CHEB / -3.8680000e+00 1.6921000e-01 9.9579000e-02 /
CHEB / -2.2202000e+00 -2.6711000e-01 3.4595000e-02 /
CHEB / -1.0384000e+00 -2.9495000e-01 -2.0037000e-02 /

C4H9O-3(+m)=C4H9O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration exact:  Others-R2H_S
C_rad_out_H/NonDeC     Cs_H_out_H/NonDeC        deltaHrxn(T=298K) = -
1.1997535550219531 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5541000e+00 2.0414000e+00 -5.3690000e-01 /
CHEB / 8.0978000e+00 1.1828000e+00 1.9798000e-01 /
CHEB / -3.2996000e+00 1.9304000e-01 1.4618000e-01 /
CHEB / -1.9226000e+00 -2.6211000e-01 4.4570000e-02 /
CHEB / -9.5485000e-01 -3.0667000e-01 -2.8223000e-02 /

C4H9O-5(+m)=C4H9O-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration exact:  R5H_SSSS
O_rad_out     Cs_H_out_2H           deltaHrxn(T=298K) = -
2.839757518331451 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.8054000e+00 2.1566000e+00 -3.2413000e-01 /
CHEB / 2.0760000e-01 6.7615000e-01 1.7529000e-01 /
CHEB / -4.8354000e+00 -1.5736000e-01 3.1551000e-02 /
CHEB / -2.2979000e+00 -3.6743000e-01 -2.2430000e-02 /
CHEB / -8.0585000e-01 -2.3788000e-01 -3.2405000e-02 /

C4H9O-5(+m)=C4H9O-3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R3H_SS    O_rad_out     Cs_H_out_H/(NonDeC/Cs)
      deltaHrxn(T=298K) = -5.069760344273428 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9988000e+00 2.4422000e+00 -3.9584000e-01 /
CHEB / 4.1445000e+00 1.3212000e+00 1.7642000e-01 /
CHEB / -4.4543000e+00 8.2525000e-03 7.0224000e-02 /
CHEB / -2.2414000e+00 -3.9610000e-01 2.2490000e-02 /
CHEB / -8.2761000e-01 -2.6233000e-01 6.2600000e-03 /

C4H9O-5(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    O_rad_out     Cs_H_out_H/(NonDeC/Cs)
      deltaHrxn(T=298K) = -9.698996193674803 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9414000e+00 1.0146000e+00 -2.6288000e-01 /
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CHEB / 1.6426000e+00 1.5041000e+00 2.4953000e-01 /
CHEB / -4.6246000e+00 8.1772000e-02 7.3117000e-02 /
CHEB / -2.3859000e+00 -3.5454000e-01 1.2760000e-02 /
CHEB / -9.0433000e-01 -2.7337000e-01 -8.5569000e-03 /

C4H9O-5(+m)=C4H9O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
R4H_SSS     O_rad_out     Cs_H_out_H/NonDeC           deltaHrxn(T=298K)
= -6.269513899295381 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5871000e+00 2.8247000e+00 -3.8042000e-01 /
CHEB / 1.6412000e+00 5.0500000e-01 2.1023000e-01 /
CHEB / -4.3607000e+00 -1.7857000e-01 5.1107000e-02 /
CHEB / -2.0344000e+00 -3.3644000e-01 -2.5833000e-02 /
CHEB / -7.4279000e-01 -2.1199000e-01 -4.0130000e-02 /

C4H9O-5(+m)=C4H7-14+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = 3.8594344389765283
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4930000e+01 6.7149000e+00 -1.2828000e+00 /
CHEB / 1.3634000e+01 1.4279000e+00 7.1923000e-01 /
CHEB / -4.1393000e+00 -2.5228000e-02 4.7608000e-01 /
CHEB / -1.7955000e+00 -4.3485000e-01 1.5452000e-01 /
CHEB / -6.2448000e-01 -2.3364000e-01 -1.2411000e-02 /

C4H9O-2(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R3H_SS    C_rad_out_H/NonDeC     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -3.4294822943794223 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0248000e+00 9.9078000e-01 -1.5557000e-01 /
CHEB / 6.4976000e+00 1.2820000e+00 -7.0726000e-02 /
CHEB / -3.3253000e+00 3.5732000e-01 7.8697000e-02 /
CHEB / -1.9992000e+00 -1.8361000e-01 6.0787000e-02 /
CHEB / -9.8785000e-01 -2.9849000e-01 -1.4160000e-02 /

C2H4+C2H5O-1(+m)=C4H9O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H2     C_rad/H2/Cs         deltaHrxn(T=298K) = -
24.02755854276065 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0110000e+00 7.4992000e-01 -1.0271000e-01 /
CHEB / -8.7338000e-01 1.1535000e+00 -9.6687000e-02 /
CHEB / -2.4617000e+00 5.1275000e-01 4.0794000e-02 /
CHEB / -1.5671000e+00 2.1534000e-02 7.8275000e-02 /
CHEB / -7.8205000e-01 -1.6338000e-01 3.1538000e-02 /

C2H4+C2H5O-1(+m)=C4H9O-3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -26.257561368702632
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.8663000e+00 1.6545000e-01 -3.4481000e-01 /
CHEB / 2.5982000e+00 2.1774000e+00 4.9151000e-02 /
CHEB / -2.0049000e+00 5.5164000e-01 1.6682000e-01 /
CHEB / -1.4187000e+00 -1.2587000e-01 7.5373000e-02 /
CHEB / -7.2842000e-01 -2.2012000e-01 -1.1289000e-02 /

C2H4+C2H5O-1(+m)=C4H9O-5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -21.187801024429202
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5826000e+00 1.4259000e+00 -3.1052000e-01 /
CHEB / -1.9599000e+00 1.3543000e+00 1.3037000e-01 /
CHEB / -3.0775000e+00 2.3810000e-01 4.0074000e-02 /
CHEB / -1.5837000e+00 -1.3018000e-01 4.2553000e-02 /
CHEB / -5.8270000e-01 -1.3198000e-01 1.7282000e-02 /

C2H4+C2H5O-1(+m)=C4H9O-4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -30.886797218104007
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0689000e+00 -5.6679000e-01 -1.5515000e-01 /
CHEB / 3.7808000e-01 2.0410000e+00 -6.7231000e-02 /
CHEB / -2.3274000e+00 7.5342000e-01 1.3839000e-01 /
CHEB / -1.6566000e+00 -1.8954000e-02 1.1369000e-01 /
CHEB / -8.5650000e-01 -2.2174000e-01 1.1545000e-02 /

C2H4+C2H5O-1(+m)=C4H9O-2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -27.45731492372458
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1890000e+00 1.6027000e-01 -3.1139000e-01 /
CHEB / 3.3028000e+00 2.2914000e+00 -1.7647000e-02 /
CHEB / -1.7910000e+00 5.8216000e-01 2.1505000e-01 /
CHEB / -1.3885000e+00 -8.6940000e-02 9.0371000e-02 /
CHEB / -7.6729000e-01 -2.3421000e-01 -7.2318000e-03 /

C2H4+C2H5O-1(+m)=C4H7-14+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -17.32836658545267
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6105000e+00 -3.5967000e-01 -1.9509000e-01 /
CHEB / 1.5059000e+01 3.9863000e-01 2.0354000e-01 /
CHEB / 2.8135000e-01 4.0758000e-02 3.6084000e-02 /
CHEB / 8.1905000e-02 -7.0264000e-02 -3.1271000e-02 /
CHEB / 3.5658000e-02 -2.7626000e-02 -2.1591000e-02 /

C2H4+C2H5O-1(+m)=CH3+C3H6O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O-1) deltaHrxn(T=298K) = -1.4404674451568162
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4032000e+00 -1.7502000e+00 -2.7584000e-01 /
CHEB / 7.2208000e+00 1.8536000e+00 1.6846000e-01 /
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CHEB / 2.3852000e-01 2.0531000e-01 1.6696000e-01 /
CHEB / -1.4371000e-01 -1.9370000e-01 1.3010000e-02 /
CHEB / -4.5010000e-02 -1.2950000e-01 -4.5135000e-02 /

C2H4+C2H5O-1(+m)=C3H7-1+CH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -8.768957727704592
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2183000e+00 -1.2517000e+00 -1.4102000e-01 /
CHEB / 4.2137000e+00 1.2512000e+00 6.5482000e-02 /
CHEB / 2.4112000e-01 2.4330000e-01 8.2534000e-02 /
CHEB / 1.1581000e-02 -1.2225000e-01 4.9516000e-02 /
CHEB / 7.7783000e-02 -1.2859000e-01 -2.0312000e-02 /

C2H4+C2H5O-1(+m)=nC4H8O+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -5.089995796841741
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1050000e+00 -2.3033000e+00 -1.7604000e-01 /
CHEB / 4.8010000e+00 2.1812000e+00 -5.8482000e-03 /
CHEB / -3.1898000e-02 5.5373000e-01 1.9582000e-01 /
CHEB / -2.6353000e-01 -1.7105000e-01 8.7399000e-02 /
CHEB / -5.1548000e-02 -2.2007000e-01 -3.3288000e-02 /

C2H4+C2H5O-1(+m)=C2H5+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -7.4492523094060985
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8204000e+00 -2.2869000e+00 -1.7931000e-01 /
CHEB / 5.3567000e+00 2.1815000e+00 -1.8045000e-03 /
CHEB / 1.0823000e-01 5.3620000e-01 1.9845000e-01 /
CHEB / -2.0923000e-01 -1.7907000e-01 8.4277000e-02 /
CHEB / -2.8978000e-02 -2.1774000e-01 -3.5887000e-02 /

C2H4+C2H5O-1(+m)=C3H6+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -5.359415349276109
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5824000e+00 -1.8828000e+00 -2.8558000e-01 /
CHEB / 6.5976000e+00 1.8949000e+00 1.3749000e-01 /
CHEB / -1.9270000e-02 3.2374000e-01 2.0256000e-01 /
CHEB / -3.3599000e-01 -1.6727000e-01 3.8932000e-02 /
CHEB / -1.6171000e-01 -1.5621000e-01 -4.8243000e-02 /

C4H8O-enol3+H(+m)=C4H9O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/Nd_Cd/H2     H_rad       deltaHrxn(T=298K) = -32.45640901637285
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2555000e+00 1.0933000e+00 -1.9777000e-01 /
CHEB / -2.8645000e+00 1.5228000e+00 -1.3398000e-01 /
CHEB / -2.8643000e+00 5.9710000e-01 7.4669000e-02 /
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CHEB / -1.6638000e+00 -1.6741000e-03 9.9652000e-02 /
CHEB / -7.8451000e-01 -1.8927000e-01 2.9187000e-02 /

C4H8O-enol3+H(+m)=C4H9O-3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -34.686411842314826
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2380000e+00 7.8449000e-01 -4.6886000e-01 /
CHEB / -4.0072000e-01 2.2297000e+00 1.3120000e-01 /
CHEB / -2.2239000e+00 4.9385000e-01 1.6441000e-01 /
CHEB / -1.4446000e+00 -1.3274000e-01 5.8474000e-02 /
CHEB / -7.0529000e-01 -2.0784000e-01 -1.3216000e-02 /

C4H8O-enol3+H(+m)=C4H9O-5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -29.6166514980414
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2032000e+00 2.2315000e+00 -3.1470000e-01 /
CHEB / -4.2028000e+00 1.2163000e+00 4.2213000e-02 /
CHEB / -3.3316000e+00 2.7294000e-01 5.7360000e-02 /
CHEB / -1.5759000e+00 -1.5194000e-01 5.8117000e-02 /
CHEB / -5.3936000e-01 -1.5405000e-01 1.8865000e-02 /

C4H8O-enol3+H(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -39.31564769171621
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8479000e+00 3.6986000e-02 -3.0227000e-01 /
CHEB / -1.7696000e+00 2.4412000e+00 -5.2156000e-02 /
CHEB / -2.6171000e+00 7.7170000e-01 1.5029000e-01 /
CHEB / -1.6510000e+00 -5.6881000e-02 8.3478000e-02 /
CHEB / -8.0352000e-01 -2.3080000e-01 -1.1875000e-02 /

C4H8O-enol3+H(+m)=C4H9O-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H/Nd     H_rad       deltaHrxn(T=298K) = -35.88616539733678
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0507000e+01 1.2038000e+00 -2.7235000e-01 /
CHEB / -2.3474000e+00 1.1078000e+00 4.1856000e-02 /
CHEB / -2.1064000e+00 4.1532000e-01 9.3492000e-02 /
CHEB / -1.2691000e+00 -1.2781000e-03 6.3682000e-02 /
CHEB / -6.8060000e-01 -1.3260000e-01 7.4297000e-03 /

C4H8O-enol3+H(+m)=C2H4+C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -8.428850473612199
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0110000e+01 -1.1308000e+00 -1.0737000e-01 /
CHEB / 2.8355000e+00 1.0862000e+00 2.6771000e-03 /
CHEB / 8.7841000e-02 2.6765000e-01 1.1566000e-01 /
CHEB / -1.2173000e-01 -1.0016000e-01 5.1224000e-02 /
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CHEB / -4.3094000e-02 -1.1721000e-01 -2.4460000e-02 /

C4H8O-enol3+H(+m)=C4H7-14+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -25.75721705906487
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4098000e+00 -3.8969000e-01 -1.9792000e-01 /
CHEB / 1.1866000e+01 4.2521000e-01 2.0161000e-01 /
CHEB / 2.1340000e-01 4.7524000e-02 3.9959000e-02 /
CHEB / 7.1788000e-02 -7.0025000e-02 -2.8331000e-02 /
CHEB / 3.8121000e-02 -2.8994000e-02 -2.1701000e-02 /

C4H8O-enol3+H(+m)=CH3+C3H6O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O-1) deltaHrxn(T=298K) = -9.869317918769017
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3725000e+00 -1.4228000e+00 -3.1320000e-01 /
CHEB / 4.4067000e+00 1.5600000e+00 2.5289000e-01 /
CHEB / 1.6993000e-01 9.7943000e-02 1.2430000e-01 /
CHEB / -1.3640000e-01 -1.6646000e-01 -1.0431000e-02 /
CHEB / -4.2646000e-02 -8.6364000e-02 -3.9630000e-02 /

C4H8O-enol3+H(+m)=C4H8O-enol2+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -1.7698371261645605
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7844000e+00 -8.5745000e-01 -1.8748000e-01 /
CHEB / 2.6304000e+00 8.5591000e-01 1.1936000e-01 /
CHEB / 1.5537000e-01 1.4593000e-01 1.0239000e-01 /
CHEB / -1.2232000e-01 -6.5673000e-02 1.2169000e-02 /
CHEB / -6.7841000e-02 -6.6591000e-02 -2.5945000e-02 /

C4H8O-enol3+H(+m)=C4H8-1+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -5.619239168011553
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4192000e+00 -1.4950000e+00 -3.1331000e-01 /
CHEB / 3.8117000e+00 1.6123000e+00 2.4296000e-01 /
CHEB / 4.7378000e-02 1.3500000e-01 1.3278000e-01 /
CHEB / -1.8059000e-01 -1.6789000e-01 -3.8988000e-03 /
CHEB / -5.8546000e-02 -9.7677000e-02 -3.9634000e-02 /

C4H8O-enol3+H(+m)=C4H8O-enol+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -6.329391019884731
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9876000e+00 -1.8857000e+00 -2.4837000e-01 /
CHEB / 3.8376000e+00 2.0216000e+00 1.1960000e-01 /
CHEB / 2.1044000e-01 2.1335000e-01 1.9296000e-01 /
CHEB / -1.0006000e-01 -2.4772000e-01 1.6520000e-02 /
CHEB / -1.8937000e-02 -1.3608000e-01 -5.7603000e-02 /
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C4H8O-enol3+H(+m)=C3H7-1+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -17.19780820131679
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9438000e+00 -9.9304000e-01 -1.5905000e-01 /
CHEB / 1.8744000e+00 1.0360000e+00 9.7740000e-02 /
CHEB / 9.4227000e-02 1.4607000e-01 8.7634000e-02 /
CHEB / -2.2129000e-02 -1.2033000e-01 2.0968000e-02 /
CHEB / 4.2298000e-02 -8.3888000e-02 -2.8672000e-02 /

C4H8O-enol3+H(+m)=nC4H8O+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -13.518846270453942
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5797000e+00 -2.0036000e+00 -2.4664000e-01 /
CHEB / 2.7656000e+00 2.0577000e+00 9.3532000e-02 /
CHEB / -1.0723000e-01 3.2902000e-01 2.0571000e-01 /
CHEB / -2.3118000e-01 -2.3021000e-01 4.2073000e-02 /
CHEB / -7.5299000e-02 -1.7097000e-01 -5.5021000e-02 /

C4H8O-enol3+H(+m)=C2H5+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -15.878102783018296
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3254000e+00 -1.9918000e+00 -2.4762000e-01 /
CHEB / 3.2963000e+00 2.0548000e+00 9.6578000e-02 /
CHEB / 3.3142000e-02 3.1686000e-01 2.0554000e-01 /
CHEB / -1.8201000e-01 -2.3266000e-01 3.9006000e-02 /
CHEB / -5.5807000e-02 -1.6749000e-01 -5.6133000e-02 /

C4H8O-enol3+H(+m)=C3H6+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -13.788265822888308
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1531000e+01 -9.3039000e-01 -1.8037000e-01 /
CHEB / 1.0260000e+00 8.9277000e-01 1.0210000e-01 /
CHEB / -1.7771000e-01 2.0002000e-01 1.0468000e-01 /
CHEB / -2.2465000e-01 -6.1409000e-02 2.5819000e-02 /
CHEB / -1.1650000e-01 -7.8120000e-02 -2.3183000e-02 /

C4H7-14+H2O(+m)=C4H9O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: 1,3_Insertion_ROR exact:
Cd/H/Nd_Cd/H2     H_OH        deltaHrxn(T=298K) = -6.699191957307981
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9832000e+01 5.6001000e+00 -1.2858000e+00 /
CHEB / 1.4325000e+01 1.8165000e+00 6.8095000e-01 /
CHEB / -3.4011000e+00 2.4692000e-01 4.4754000e-01 /
CHEB / -1.7779000e+00 -3.2073000e-01 1.4011000e-01 /
CHEB / -8.2448000e-01 -2.4811000e-01 -2.7407000e-02 /
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C4H7-14+H2O(+m)=C4H9O-3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -8.929194783249958
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2213000e+01 5.9521000e+00 -1.3730000e+00 /
CHEB / 1.6097000e+01 1.5598000e+00 8.2782000e-01 /
CHEB / -2.6421000e+00 1.3056000e-01 4.7084000e-01 /
CHEB / -1.4252000e+00 -3.4852000e-01 1.2221000e-01 /
CHEB / -7.0546000e-01 -2.3542000e-01 -4.4328000e-02 /

C4H7-14+H2O(+m)=C4H9O-4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -13.558430632651334
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0939000e+01 4.9310000e+00 -1.3949000e+00 /
CHEB / 1.4767000e+01 2.2204000e+00 8.3530000e-01 /
CHEB / -3.2197000e+00 3.6189000e-01 4.4437000e-01 /
CHEB / -1.7196000e+00 -2.5262000e-01 1.1785000e-01 /
CHEB / -8.2555000e-01 -2.0733000e-01 -3.9328000e-02 /

C4H7-14+H2O(+m)=C4H9O-2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -10.128948338271911
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1437000e+01 6.1115000e+00 -1.5214000e+00 /
CHEB / 1.6855000e+01 1.3719000e+00 8.6022000e-01 /
CHEB / -2.3960000e+00 1.1241000e-01 4.6335000e-01 /
CHEB / -1.3972000e+00 -3.1798000e-01 9.2763000e-02 /
CHEB / -7.6188000e-01 -2.0219000e-01 -6.2100000e-02 /

CH3+C3H6O-enol2(+m)=C4H9O-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -22.587091097603835
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1624000e+00 3.0332000e-01 -3.6081000e-01 /
CHEB / 1.8596000e+00 2.4228000e+00 -1.6729000e-02 /
CHEB / -2.6874000e+00 6.2672000e-01 1.5716000e-01 /
CHEB / -1.7297000e+00 -1.2505000e-01 8.2923000e-02 /
CHEB / -8.2016000e-01 -2.3973000e-01 -3.1573000e-03 /

CH3+C3H6O-enol2(+m)=C4H9O-3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond exact:
C_methyl     Cd/H2_Cd/H/Nd          deltaHrxn(T=298K) = -
24.817093923545812 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9196000e+00 9.7726000e-01 -1.3965000e-01 /
CHEB / -8.6860000e-01 1.1732000e+00 -5.9144000e-03 /
CHEB / -2.4755000e+00 3.6702000e-01 8.3619000e-02 /
CHEB / -1.3947000e+00 -5.0022000e-02 4.5461000e-02 /
CHEB / -6.7979000e-01 -1.3666000e-01 -5.6352000e-03 /
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CH3+C3H6O-enol2(+m)=C4H9O-5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -19.747333579272386
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0638000e+00 1.4767000e+00 -3.4515000e-01 /
CHEB / 4.8275000e-01 2.2213000e+00 8.9144000e-02 /
CHEB / -3.2964000e+00 2.9435000e-01 8.9746000e-02 /
CHEB / -1.6694000e+00 -1.8518000e-01 8.6531000e-02 /
CHEB / -5.7763000e-01 -1.4293000e-01 3.0176000e-02 /

CH3+C3H6O-enol2(+m)=C4H9O-4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -29.446329772947188
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4981000e+00 3.4318000e-01 -2.3834000e-01 /
CHEB / 1.9839000e+00 2.3266000e+00 4.1978000e-02 /
CHEB / -2.7460000e+00 4.9388000e-01 1.3227000e-01 /
CHEB / -1.6943000e+00 -1.0414000e-01 2.7854000e-02 /
CHEB / -8.0853000e-01 -1.7448000e-01 -1.3052000e-02 /

CH3+C3H6O-enol2(+m)=C4H9O-2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -26.016847478567765
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9168000e+00 9.4346000e-01 -5.5331000e-01 /
CHEB / 2.7950000e+00 2.1051000e+00 2.2348000e-01 /
CHEB / -2.0099000e+00 4.5674000e-01 1.7933000e-01 /
CHEB / -1.3425000e+00 -1.1787000e-01 4.8457000e-02 /
CHEB / -7.1636000e-01 -1.8492000e-01 -1.8108000e-02 /

CH3+C3H6O-enol2(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -15.887899140295858
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7963000e+00 -4.5783000e-01 -2.4415000e-01 /
CHEB / 1.5853000e+01 5.0910000e-01 2.5813000e-01 /
CHEB / 3.7092000e-01 4.2673000e-02 3.7294000e-02 /
CHEB / 1.1294000e-01 -8.2864000e-02 -3.7076000e-02 /
CHEB / 3.9872000e-02 -3.0006000e-02 -2.2664000e-02 /

CH3+C3H6O-enol2(+m)=C3H7-1+CH2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -7.328490282547772
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3547000e+00 -1.3582000e+00 -1.2999000e-01 /
CHEB / 7.0276000e+00 1.6683000e+00 1.1160000e-01 /
CHEB / 3.8457000e-01 -1.1988000e-01 4.1542000e-02 /
CHEB / 1.2083000e-01 -1.9030000e-01 5.5756000e-03 /
CHEB / 7.1419000e-02 -4.9501000e-02 -2.6962000e-02 /
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CH3+C3H6O-enol2(+m)=nC4H8O+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -3.6495283516849284
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7310000e+00 -1.5809000e+00 -2.6311000e-01 /
CHEB / 6.7339000e+00 1.7902000e+00 1.9125000e-01 /
CHEB / -1.6996000e-02 6.6197000e-02 1.4564000e-01 /
CHEB / -1.2122000e-01 -2.2464000e-01 -2.0928000e-02 /
CHEB / -1.4796000e-02 -9.6083000e-02 -4.8692000e-02 /

CH3+C3H6O-enol2(+m)=C2H5+C2H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -6.008784864249279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4947000e+00 -1.5650000e+00 -2.6592000e-01 /
CHEB / 7.2524000e+00 1.7783000e+00 1.9660000e-01 /
CHEB / 1.1999000e-01 5.7581000e-02 1.4402000e-01 /
CHEB / -7.5760000e-02 -2.2373000e-01 -2.2986000e-02 /
CHEB / 4.7327000e-04 -9.2620000e-02 -4.8872000e-02 /

C4H8O-enol2+H(+m)=C4H9O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -30.686571890208292
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9628000e+00 3.2059000e-01 -3.7668000e-01 /
CHEB / -1.5903000e-01 2.4361000e+00 -2.6944000e-02 /
CHEB / -2.6408000e+00 6.2797000e-01 1.9540000e-01 /
CHEB / -1.7699000e+00 -1.4365000e-01 1.0858000e-01 /
CHEB / -8.5594000e-01 -2.7204000e-01 1.1058000e-03 /

C4H8O-enol2+H(+m)=C4H9O-3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/H/Nd     H_rad      deltaHrxn(T=298K) = -
32.916574716150265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5413000e+00 1.1684000e+00 -1.9846000e-01 /
CHEB / -2.8925000e+00 1.2343000e+00 2.2758000e-02 /
CHEB / -2.5097000e+00 3.6654000e-01 9.5579000e-02 /
CHEB / -1.4236000e+00 -5.3762000e-02 4.4171000e-02 /
CHEB / -6.8681000e-01 -1.3454000e-01 -8.0727000e-03 /

C4H8O-enol2+H(+m)=C4H9O-5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -27.84681437187684
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3071000e+00 2.3758000e+00 -3.8199000e-01 /
CHEB / -3.8138000e+00 1.1164000e+00 1.5287000e-01 /
CHEB / -3.1515000e+00 8.3747000e-02 7.3480000e-02 /
CHEB / -1.5212000e+00 -1.8328000e-01 2.2836000e-02 /
CHEB / -5.5444000e-01 -1.1735000e-01 -5.1681000e-03 /
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C4H8O-enol2+H(+m)=C4H9O-4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -37.54581056555165
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7884000e+00 2.4318000e-01 -3.8153000e-01 /
CHEB / -1.1919000e+00 2.3741000e+00 -4.3710000e-03 /
CHEB / -2.4481000e+00 5.9553000e-01 1.9052000e-01 /
CHEB / -1.6138000e+00 -1.4210000e-01 8.1595000e-02 /
CHEB / -8.1206000e-01 -2.3493000e-01 -2.1930000e-02 /

C4H8O-enol2+H(+m)=C4H9O-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/H/Nd     H_rad      deltaHrxn(T=298K) = -
34.11632827117222 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0068000e+01 1.0701000e+00 -2.2237000e-01 /
CHEB / -2.1435000e+00 1.1009000e+00 1.3696000e-02 /
CHEB / -2.1082000e+00 4.1521000e-01 8.6415000e-02 /
CHEB / -1.2894000e+00 3.5733000e-03 6.3111000e-02 /
CHEB / -7.0280000e-01 -1.2974000e-01 8.6277000e-03 /

C4H8O-enol2+H(+m)=C2H4+C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -6.6590133474476385
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1068000e+00 -1.7635000e+00 -3.0252000e-01 /
CHEB / 5.3739000e+00 1.8270000e+00 1.7473000e-01 /
CHEB / 1.1667000e-01 2.4915000e-01 1.9111000e-01 /
CHEB / -2.6812000e-01 -1.8051000e-01 2.2186000e-02 /
CHEB / -1.2214000e-01 -1.3662000e-01 -5.2557000e-02 /

C4H8O-enol2+H(+m)=C4H7-14+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -23.98737993290031
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5462000e+00 -5.5092000e-01 -2.9296000e-01 /
CHEB / 1.3392000e+01 6.0334000e-01 3.0317000e-01 /
CHEB / 2.5567000e-01 6.4089000e-02 5.3586000e-02 /
CHEB / -1.1175000e-03 -9.8722000e-02 -4.3762000e-02 /
CHEB / -6.1216000e-03 -4.0036000e-02 -2.9645000e-02 /

C4H8O-enol2+H(+m)=CH3+C3H6O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O-1) deltaHrxn(T=298K) = -8.099480792604457
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0675000e+01 -8.0195000e-01 -1.6052000e-01 /
CHEB / 2.2017000e+00 9.0290000e-01 1.2018000e-01 /
CHEB / -4.2388000e-03 3.9607000e-02 8.6175000e-02 /
CHEB / -1.1177000e-01 -1.1371000e-01 -1.4981000e-02 /
CHEB / -2.8168000e-02 -4.8811000e-02 -3.1042000e-02 /
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C4H8O-enol2+H(+m)=C4H8-1+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -3.849402041846993
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0915000e+01 -8.7151000e-01 -1.5231000e-01 /
CHEB / 1.4210000e+00 9.4938000e-01 1.0063000e-01 /
CHEB / -1.4673000e-01 8.5284000e-02 9.3028000e-02 /
CHEB / -1.4957000e-01 -1.2053000e-01 -4.0229000e-03 /
CHEB / -4.0796000e-02 -6.4139000e-02 -3.2037000e-02 /

C4H8O-enol2+H(+m)=C4H8O-enol+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -4.559553893720171
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4860000e+00 -8.5943000e-01 -1.5411000e-01 /
CHEB / 2.3234000e+00 9.4001000e-01 1.0366000e-01 /
CHEB / 9.2299000e-02 7.6338000e-02 9.2135000e-02 /
CHEB / -6.9038000e-02 -1.1706000e-01 -5.5488000e-03 /
CHEB / -1.2677000e-02 -5.9393000e-02 -3.1317000e-02 /

C4H8O-enol2+H(+m)=C3H7-1+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -15.427971075152229
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0811000e+00 -8.8984000e-01 -2.0623000e-01 /
CHEB / 2.4385000e+00 9.5127000e-01 1.6037000e-01 /
CHEB / 2.4358000e-01 8.6947000e-02 8.6068000e-02 /
CHEB / 1.8585000e-02 -9.1357000e-02 2.4729000e-04 /
CHEB / 5.0990000e-02 -6.1982000e-02 -2.8530000e-02 /

C4H8O-enol2+H(+m)=nC4H8O+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -11.749009144289381
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5711000e+00 -1.8482000e+00 -2.9711000e-01 /
CHEB / 3.4134000e+00 1.9295000e+00 1.6044000e-01 /
CHEB / -3.0896000e-02 2.4763000e-01 2.0704000e-01 /
CHEB / -2.7527000e-01 -2.0154000e-01 1.7169000e-02 /
CHEB / -1.1658000e-01 -1.3515000e-01 -5.9135000e-02 /

C4H8O-enol2+H(+m)=C2H5+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -14.108265656853735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3145000e+00 -1.8344000e+00 -2.9852000e-01 /
CHEB / 3.9477000e+00 1.9232000e+00 1.6449000e-01 /
CHEB / 1.0647000e-01 2.3657000e-01 2.0591000e-01 /
CHEB / -2.2715000e-01 -2.0291000e-01 1.4236000e-02 /
CHEB / -9.7283000e-02 -1.3224000e-01 -5.9527000e-02 /
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C4H8O-enol2+H(+m)=C3H6+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -12.018428696723747
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0907000e+01 -9.7488000e-01 -1.6568000e-01 /
CHEB / 1.2535000e+00 9.3227000e-01 8.1312000e-02 /
CHEB / -2.1172000e-01 2.1118000e-01 1.0731000e-01 /
CHEB / -2.6575000e-01 -6.1970000e-02 3.0062000e-02 /
CHEB / -1.4630000e-01 -8.1645000e-02 -2.2180000e-02 /

C4H8-1+OH(+m)=C4H9O-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -26.8371698483613
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1729000e+00 7.6246000e-02 -3.2533000e-01 /
CHEB / 6.4458000e-02 2.2535000e+00 -1.4665000e-02 /
CHEB / -2.6861000e+00 6.2395000e-01 1.4479000e-01 /
CHEB / -1.7387000e+00 -1.1598000e-01 8.2351000e-02 /
CHEB / -8.3478000e-01 -2.3771000e-01 -2.2470000e-03 /

C4H8-1+OH(+m)=C4H9O-3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H2_Cd/H/Nd     O_pri_rad          deltaHrxn(T=298K) = -
29.067172674303276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0793000e+01 6.5843000e-01 -5.1710000e-02 /
CHEB / -3.4871000e+00 9.7246000e-01 -2.2483000e-02 /
CHEB / -2.3533000e+00 3.7718000e-01 5.4173000e-02 /
CHEB / -1.3963000e+00 -1.4525000e-02 4.4700000e-02 /
CHEB / -6.9446000e-01 -1.2556000e-01 1.5555000e-03 /

C4H8-1+OH(+m)=C4H9O-5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -23.997412330029846
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0801000e+00 1.2104000e+00 -3.3338000e-01 /
CHEB / -1.2835000e+00 2.1114000e+00 1.2383000e-01 /
CHEB / -3.2997000e+00 2.9310000e-01 7.7410000e-02 /
CHEB / -1.6910000e+00 -1.9168000e-01 7.3988000e-02 /
CHEB / -5.9235000e-01 -1.3719000e-01 3.2399000e-02 /

C4H8-1+OH(+m)=C4H9O-4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -33.69640852370465
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4376000e+00 7.1679000e-02 -1.8486000e-01 /
CHEB / 2.7902000e-01 2.2126000e+00 2.0291000e-02 /
CHEB / -2.7614000e+00 4.8597000e-01 1.3032000e-01 /
CHEB / -1.7143000e+00 -1.0025000e-01 3.2033000e-02 /
CHEB / -8.2523000e-01 -1.7755000e-01 -1.3231000e-02 /
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C4H8-1+OH(+m)=C4H9O-2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -30.26692622932523
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8768000e+00 6.9890000e-01 -5.2044000e-01 /
CHEB / 1.0199000e+00 1.9805000e+00 2.1910000e-01 /
CHEB / -2.0489000e+00 4.7887000e-01 1.7134000e-01 /
CHEB / -1.3646000e+00 -1.0724000e-01 4.9408000e-02 /
CHEB / -7.2924000e-01 -1.8773000e-01 -1.7914000e-02 /

C4H8-1+OH(+m)=C2H4+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -2.8096113056006455
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9033000e+00 -1.8380000e+00 -2.6630000e-01 /
CHEB / 5.4720000e+00 1.9025000e+00 1.4827000e-01 /
CHEB / 4.1717000e-02 2.6234000e-01 1.7056000e-01 /
CHEB / -2.2429000e-01 -1.8714000e-01 2.4075000e-02 /
CHEB / -7.6920000e-02 -1.4296000e-01 -4.1779000e-02 /

C4H8-1+OH(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -20.137977891053318
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5457000e+00 -4.3384000e-01 -2.4068000e-01 /
CHEB / 1.4229000e+01 4.8393000e-01 2.5582000e-01 /
CHEB / 2.6588000e-01 4.1285000e-02 3.6511000e-02 /
CHEB / 5.3206000e-02 -8.1197000e-02 -3.7896000e-02 /
CHEB / 1.6353000e-02 -2.9666000e-02 -2.2848000e-02 /

C4H8-1+OH(+m)=CH3+C3H6O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -4.2500787507574636
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0567000e+01 -9.3785000e-01 -1.3278000e-01 /
CHEB / 2.1167000e+00 1.0067000e+00 7.0940000e-02 /
CHEB / -1.8347000e-01 1.0931000e-01 9.8738000e-02 /
CHEB / -1.8018000e-01 -1.2556000e-01 3.7636000e-03 /
CHEB / -5.4129000e-02 -7.3427000e-02 -3.1894000e-02 /

C4H8-1+OH(+m)=C3H7-1+CH2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -11.578569033305236
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9665000e+00 -1.4754000e+00 -1.3593000e-01 /
CHEB / 5.0385000e+00 1.7833000e+00 1.2001000e-01 /
CHEB / 2.6445000e-01 -8.8307000e-02 3.4466000e-02 /
CHEB / 6.2663000e-02 -2.0797000e-01 1.1422000e-02 /
CHEB / 6.2139000e-02 -6.4304000e-02 -2.4384000e-02 /
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C4H8-1+OH(+m)=nC4H8O+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -7.899607102442388
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4094000e+00 -1.6937000e+00 -2.3821000e-01 /
CHEB / 4.7788000e+00 1.8679000e+00 1.5278000e-01 /
CHEB / -1.6179000e-01 1.2913000e-01 1.5052000e-01 /
CHEB / -1.9517000e-01 -2.2518000e-01 -8.1903000e-03 /
CHEB / -4.1411000e-02 -1.1760000e-01 -4.4987000e-02 /

C4H8-1+OH(+m)=C2H5+C2H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -10.258863615006742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1659000e+00 -1.6745000e+00 -2.4216000e-01 /
CHEB / 5.2994000e+00 1.8553000e+00 1.5928000e-01 /
CHEB / -2.1819000e-02 1.1783000e-01 1.4951000e-01 /
CHEB / -1.4774000e-01 -2.2577000e-01 -1.0619000e-02 /
CHEB / -2.5182000e-02 -1.1369000e-01 -4.5711000e-02 /

C4H8-1+OH(+m)=C3H6+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -8.169026654876754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3615000e+00 -1.4880000e+00 -3.6451000e-01 /
CHEB / 4.3274000e+00 1.5881000e+00 2.9193000e-01 /
CHEB / -1.5557000e-01 1.4552000e-01 1.4626000e-01 /
CHEB / -2.8096000e-01 -1.5451000e-01 -1.0441000e-02 /
CHEB / -1.3167000e-01 -8.9453000e-02 -4.3352000e-02 /

C4H8O-enol+H(+m)=C4H9O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -26.12701799648812
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6233000e+00 -3.3896000e-01 -1.7692000e-01 /
CHEB / -1.0548000e+00 2.3543000e+00 -8.6671000e-02 /
CHEB / -2.6394000e+00 8.3782000e-01 1.3506000e-01 /
CHEB / -1.7462000e+00 -4.2616000e-02 9.7778000e-02 /
CHEB / -8.2946000e-01 -2.4448000e-01 -8.9763000e-03 /

C4H8O-enol+H(+m)=C4H9O-3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/H/Nd     H_rad      deltaHrxn(T=298K) = -
28.357020822430098 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0101000e+01 7.2071000e-01 -6.6274000e-02 /
CHEB / -2.5879000e+00 1.0281000e+00 -2.3406000e-02 /
CHEB / -2.3762000e+00 3.7852000e-01 6.1121000e-02 /
CHEB / -1.3953000e+00 -2.3385000e-02 4.5805000e-02 /
CHEB / -6.8412000e-01 -1.2882000e-01 -1.5235000e-04 /
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C4H8O-enol+H(+m)=C4H9O-5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -23.287260478156668
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5140000e-01 5.8476000e-01 -2.6849000e-01 /
CHEB / -2.0841000e+00 2.5402000e+00 1.3415000e-01 /
CHEB / -3.3047000e+00 4.6817000e-01 6.3528000e-02 /
CHEB / -1.7139000e+00 -1.5575000e-01 6.5751000e-02 /
CHEB / -5.8594000e-01 -1.5385000e-01 1.6553000e-02 /

C4H8O-enol+H(+m)=C4H9O-4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/H/Nd     H_rad      deltaHrxn(T=298K) = -
32.98625667183147 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4335000e+00 1.0054000e+00 -1.1603000e-01 /
CHEB / -3.2748000e+00 1.4532000e+00 -6.9476000e-02 /
CHEB / -2.9331000e+00 5.3740000e-01 8.4745000e-02 /
CHEB / -1.6719000e+00 -3.4729000e-02 7.7046000e-02 /
CHEB / -7.8721000e-01 -1.7913000e-01 4.9823000e-03 /

C4H8O-enol+H(+m)=C4H9O-2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -29.55677437745205
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0455000e+00 3.0810000e-03 -2.6681000e-01 /
CHEB / 6.1198000e-01 2.3364000e+00 1.5889000e-03 /
CHEB / -1.9950000e+00 6.2140000e-01 1.8840000e-01 /
CHEB / -1.4197000e+00 -1.0990000e-01 7.9592000e-02 /
CHEB / -7.4427000e-01 -2.1701000e-01 -2.1356000e-02 /

C4H8O-enol+H(+m)=C2H4+C2H5O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -2.0994594537274676
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7419000e+00 -2.1614000e+00 -1.9722000e-01 /
CHEB / 4.9477000e+00 2.1763000e+00 3.3742000e-02 /
CHEB / 9.5817000e-02 4.0739000e-01 2.0418000e-01 /
CHEB / -1.6891000e-01 -2.3702000e-01 5.4816000e-02 /
CHEB / -2.2154000e-02 -1.9933000e-01 -5.0662000e-02 /

C4H8O-enol+H(+m)=C4H7-14+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -19.42782603918014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1620000e+00 -6.6207000e-01 -3.4870000e-01 /
CHEB / 1.4272000e+01 7.7703000e-01 3.8410000e-01 /
CHEB / 2.6460000e-01 3.7547000e-03 3.5640000e-02 /
CHEB / 1.0947000e-01 -1.1531000e-01 -5.7471000e-02 /
CHEB / 5.4286000e-02 -3.1142000e-02 -2.8116000e-02 /
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C4H8O-enol+H(+m)=CH3+C3H6O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O-1) deltaHrxn(T=298K) = -3.5399268988842856
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0129000e+01 -9.2009000e-01 -1.3587000e-01 /
CHEB / 2.8974000e+00 9.9696000e-01 7.6501000e-02 /
CHEB / -1.3040000e-01 9.5732000e-02 9.8185000e-02 /
CHEB / -1.5654000e-01 -1.2510000e-01 4.9996000e-04 /
CHEB / -3.6611000e-02 -6.9083000e-02 -3.2318000e-02 /

C4H8O-enol+H(+m)=C4H8-1+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = 0.710151851873178
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0584000e+01 -1.0390000e+00 -1.0333000e-01 /
CHEB / 1.8826000e+00 1.0744000e+00 2.9081000e-02 /
CHEB / -2.3081000e-01 1.6675000e-01 1.0017000e-01 /
CHEB / -2.1189000e-01 -1.2608000e-01 1.8503000e-02 /
CHEB / -5.0614000e-02 -9.1291000e-02 -2.8351000e-02 /

C4H8O-enol+H(+m)=C3H7-1+CH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -10.868417181432058
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6893000e+00 -1.8999000e+00 -1.1023000e-01 /
CHEB / 4.6815000e+00 2.2124000e+00 6.0679000e-02 /
CHEB / 3.4866000e-01 3.4240000e-02 6.8364000e-02 /
CHEB / 9.8093000e-02 -3.1392000e-01 2.6983000e-02 /
CHEB / 1.0395000e-01 -1.1904000e-01 -3.5909000e-02 /

C4H8O-enol+H(+m)=nC4H8O+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -7.18945525056921
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7965000e+00 -1.0988000e+00 -9.4596000e-02 /
CHEB / 1.9384000e+00 1.1250000e+00 3.4156000e-03 /
CHEB / -2.0288000e-01 2.1061000e-01 1.1395000e-01 /
CHEB / -1.9929000e-01 -1.5143000e-01 3.5234000e-02 /
CHEB / -5.2364000e-02 -1.1631000e-01 -3.7076000e-02 /

C4H8O-enol+H(+m)=C2H5+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -9.548711763133564
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0506000e+01 -1.0902000e+00 -9.6403000e-02 /
CHEB / 2.5152000e+00 1.1236000e+00 6.0091000e-03 /
CHEB / -6.1075000e-02 2.0062000e-01 1.1524000e-01 /
CHEB / -1.5165000e-01 -1.5329000e-01 3.2719000e-02 /
CHEB / -3.4389000e-02 -1.1278000e-01 -3.8486000e-02 /
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C4H8O-enol+H(+m)=C3H6+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -7.458874803003576
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0246000e+00 -1.8946000e+00 -2.6652000e-01 /
CHEB / 4.2036000e+00 1.9945000e+00 1.2757000e-01 /
CHEB / -1.3559000e-01 2.3597000e-01 2.0438000e-01 /
CHEB / -3.1165000e-01 -2.1217000e-01 2.0450000e-02 /
CHEB / -1.2312000e-01 -1.3319000e-01 -5.5960000e-02 /

C3H7-1+CH2O(+m)=C4H9O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -15.258600815056063
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6246000e-01 6.9841000e-01 -2.0984000e-01 /
CHEB / 5.5350000e-01 1.7908000e+00 7.3714000e-02 /
CHEB / -2.9467000e+00 5.8826000e-01 5.9068000e-02 /
CHEB / -1.8255000e+00 2.5821000e-03 8.0317000e-02 /
CHEB / -8.7922000e-01 -1.7807000e-01 3.4298000e-02 /

C3H7-1+CH2O(+m)=C4H9O-3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -17.48860364099804
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5432000e+00 6.5168000e-01 -2.3750000e-01 /
CHEB / 3.9649000e+00 2.6398000e+00 1.7293000e-01 /
CHEB / -2.6132000e+00 4.6344000e-01 8.4277000e-02 /
CHEB / -1.6216000e+00 -1.2464000e-01 6.8081000e-02 /
CHEB / -7.6022000e-01 -1.5098000e-01 1.7007000e-02 /

C3H7-1+CH2O(+m)=C4H9O-5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond exact:
C_rad/H2/Cs     CO/H2_O       deltaHrxn(T=298K) = -12.418843296724612
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1639000e+00 1.1969000e+00 -9.9375000e-02 /
CHEB / -4.0263000e+00 9.5187000e-01 8.9776000e-02 /
CHEB / -3.5851000e+00 2.4870000e-02 4.6467000e-02 /
CHEB / -1.5463000e+00 -1.7273000e-01 -2.1770000e-02 /
CHEB / -4.7873000e-01 -6.7215000e-02 -2.7761000e-02 /

C3H7-1+CH2O(+m)=C4H9O-4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -22.117839490399415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5906000e+00 -3.2767000e-01 -1.5495000e-01 /
CHEB / 1.9103000e+00 2.7598000e+00 1.2530000e-01 /
CHEB / -2.8823000e+00 7.4098000e-01 8.0657000e-02 /
CHEB / -1.9015000e+00 -6.3154000e-02 7.4818000e-02 /
CHEB / -9.0950000e-01 -1.8971000e-01 1.9219000e-02 /
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C3H7-1+CH2O(+m)=C4H9O-2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -18.688357196019993
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1321000e-02 1.0301000e+00 -2.5587000e-01 /
CHEB / 1.8865000e+00 1.6902000e+00 1.1391000e-01 /
CHEB / -2.3227000e+00 4.9792000e-01 9.9327000e-02 /
CHEB / -1.4539000e+00 -1.2144000e-02 6.1029000e-02 /
CHEB / -7.7673000e-01 -1.4492000e-01 8.7027000e-03 /

C3H7-1+CH2O(+m)=C4H7-14+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -8.559408857748082
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0966000e+01 -3.9439000e-01 -1.9697000e-01 /
CHEB / 1.6958000e+01 4.3002000e-01 2.0073000e-01 /
CHEB / 2.9295000e-01 4.7207000e-02 3.9119000e-02 /
CHEB / 1.9731000e-01 -7.0409000e-02 -2.8302000e-02 /
CHEB / 1.2751000e-01 -2.8429000e-02 -2.1151000e-02 /

nC4H8O+H(+m)=C4H9O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -18.93756274591891
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2150000e+00 -7.7233000e-01 -8.7670000e-02 /
CHEB / -1.3767000e-02 1.8601000e+00 -4.3949000e-02 /
CHEB / -2.5393000e+00 7.3317000e-01 1.1874000e-01 /
CHEB / -1.7904000e+00 -3.2963000e-02 1.1226000e-01 /
CHEB / -8.6287000e-01 -2.4139000e-01 1.5683000e-02 /

nC4H8O+H(+m)=C4H9O-3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -21.167565571860887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5307000e+00 1.3080000e-01 -2.1280000e-01 /
CHEB / 3.2853000e+00 2.1367000e+00 6.3888000e-02 /
CHEB / -2.5363000e+00 4.4044000e-01 1.5637000e-01 /
CHEB / -1.5317000e+00 -1.3236000e-01 3.8052000e-02 /
CHEB / -7.3012000e-01 -1.8846000e-01 -2.1534000e-02 /

nC4H8O+H(+m)=C4H9O-5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) CO/H/Nd_O     H_rad      deltaHrxn(T=298K) = -
16.097805227587457 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0160000e-01 2.8675000e+00 -2.1929000e-01 /
CHEB / -2.3461000e+00 3.7617000e-01 2.0779000e-01 /
CHEB / -3.5948000e+00 -6.3443000e-02 1.5397000e-02 /
CHEB / -1.5263000e+00 -1.2982000e-01 -5.5645000e-02 /
CHEB / -4.5598000e-01 -3.8375000e-02 -3.2084000e-02 /
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nC4H8O+H(+m)=C4H9O-4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond Primary
Kinetic Library: Mike   deltaHrxn(T=298K) = -25.796801421262263 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8596000e+00 6.2895000e-01 -3.4760000e-02 /
CHEB / -2.5688000e+00 1.0026000e+00 -2.4240000e-02 /
CHEB / -2.6044000e+00 4.6067000e-01 4.5656000e-02 /
CHEB / -1.5721000e+00 2.0273000e-02 5.6178000e-02 /
CHEB / -7.6873000e-01 -1.4493000e-01 1.4176000e-02 /

nC4H8O+H(+m)=C4H9O-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -22.36731912688284
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2659000e+00 -3.8760000e-01 -1.9301000e-01 /
CHEB / 2.2331000e+00 2.0553000e+00 -1.9813000e-02 /
CHEB / -1.9909000e+00 6.2974000e-01 1.5955000e-01 /
CHEB / -1.4057000e+00 -8.4345000e-02 8.6942000e-02 /
CHEB / -7.4951000e-01 -2.2307000e-01 -1.3648000e-02 /

nC4H8O+H(+m)=C4H7-14+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -12.23837078861093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3522000e+00 -6.4702000e-01 -3.7144000e-01 /
CHEB / 1.6083000e+01 7.6194000e-01 4.0907000e-01 /
CHEB / 1.1759000e-02 8.9768000e-03 4.2164000e-02 /
CHEB / 4.4262000e-02 -1.2022000e-01 -6.3961000e-02 /
CHEB / 6.2484000e-02 -3.5890000e-02 -3.3174000e-02 /

nC4H8O+H(+m)=C3H7-1+CH2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -3.6789619308628474
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1904000e+00 -1.3604000e-01 -6.8605000e-02 /
CHEB / 4.0485000e+00 1.7730000e-01 9.3194000e-02 /
CHEB / -5.7279000e-03 -2.3654000e-02 -1.8417000e-02 /
CHEB / 2.3246000e-02 -2.3944000e-02 -1.0505000e-02 /
CHEB / 2.4837000e-02 3.7156000e-04 2.4307000e-03 /

nC4H8O+H(+m)=C2H5+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -2.359256512564354
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7167000e+00 -1.1834000e+00 -6.9504000e-02 /
CHEB / 3.4875000e+00 1.1373000e+00 -2.1303000e-02 /
CHEB / -1.2981000e-01 3.0413000e-01 9.2620000e-02 /
CHEB / -2.1776000e-01 -1.2833000e-01 5.3513000e-02 /
CHEB / -4.8290000e-02 -1.4472000e-01 -2.0691000e-02 /
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nC4H8O+H(+m)=C3H6+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -0.26941955243436544
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7159000e+00 -2.0770000e+00 -2.3677000e-01 /
CHEB / 5.5407000e+00 2.0698000e+00 7.0502000e-02 /
CHEB / -3.6122000e-01 3.7623000e-01 2.0958000e-01 /
CHEB / -4.2966000e-01 -1.8657000e-01 5.1193000e-02 /
CHEB / -1.8352000e-01 -1.6685000e-01 -4.8376000e-02 /

C2H5+C2H4O(+m)=C4H9O-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -16.578306233354557
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4533000e+00 -7.2490000e-01 -9.6896000e-02 /
CHEB / 1.7098000e+00 1.9160000e+00 -4.8473000e-02 /
CHEB / -2.3115000e+00 7.4105000e-01 1.2379000e-01 /
CHEB / -1.7089000e+00 -3.8285000e-02 1.1375000e-01 /
CHEB / -8.3563000e-01 -2.4273000e-01 1.4114000e-02 /

C2H5+C2H4O(+m)=C4H9O-3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -18.808309059296533
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1076000e+00 1.8007000e-01 -2.2086000e-01 /
CHEB / 4.8790000e+00 2.1601000e+00 6.9003000e-02 /
CHEB / -2.2715000e+00 4.4092000e-01 1.5791000e-01 /
CHEB / -1.4462000e+00 -1.3550000e-01 3.7118000e-02 /
CHEB / -7.0227000e-01 -1.8893000e-01 -2.2240000e-02 /

C2H5+C2H4O(+m)=C4H9O-5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -13.738548715023105
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3166000e+00 8.2591000e-02 -2.4223000e-01 /
CHEB / 1.1034000e+00 2.3666000e+00 2.0492000e-01 /
CHEB / -3.0871000e+00 4.1901000e-01 6.8868000e-02 /
CHEB / -1.6701000e+00 -1.5406000e-01 5.7398000e-02 /
CHEB / -5.8988000e-01 -1.4357000e-01 2.1350000e-02 /

C2H5+C2H4O(+m)=C4H9O-4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) C_rad/H2/Cs     Cd/H2_Cd/H/Nd        deltaHrxn(T=298K) = -
23.43754490869791 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9615000e+00 6.7782000e-01 -4.3339000e-02 /
CHEB / -7.2809000e-01 1.0697000e+00 -3.1521000e-02 /
CHEB / -2.3987000e+00 4.7772000e-01 4.9620000e-02 /
CHEB / -1.5041000e+00 1.3449000e-02 5.9699000e-02 /
CHEB / -7.4454000e-01 -1.5103000e-01 1.3238000e-02 /
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C2H5+C2H4O(+m)=C4H9O-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -20.008062614318487
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5813000e+00 -3.4385000e-01 -2.0105000e-01 /
CHEB / 3.8748000e+00 2.0915000e+00 -1.8650000e-02 /
CHEB / -1.7297000e+00 6.2854000e-01 1.6394000e-01 /
CHEB / -1.3242000e+00 -8.9392000e-02 8.6778000e-02 /
CHEB / -7.2285000e-01 -2.2379000e-01 -1.4834000e-02 /

C2H5+C2H4O(+m)=C3H7-1+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -1.3197054182984935
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7987000e-01 -2.0877000e+00 -1.2724000e-01 /
CHEB / 7.5636000e+00 2.3286000e+00 7.1914000e-02 /
CHEB / 3.6276000e-01 1.5758000e-01 6.4130000e-02 /
CHEB / 9.0599000e-02 -3.1091000e-01 4.2833000e-02 /
CHEB / 1.3221000e-01 -1.6573000e-01 -2.8286000e-02 /

C3H6+CH2OH(+m)=C4H9O-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -18.668143193484546
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5029000e-01 -1.1355000e-01 -2.3824000e-01 /
CHEB / 3.0865000e+00 2.3196000e+00 -1.0192000e-01 /
CHEB / -2.5956000e+00 5.7149000e-01 2.1160000e-01 /
CHEB / -1.7468000e+00 -1.1554000e-01 1.0463000e-01 /
CHEB / -8.5997000e-01 -2.7201000e-01 3.5627000e-03 /

C3H6+CH2OH(+m)=C4H9O-3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -20.898146019426523
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1570000e-02 5.7174000e-01 -4.8752000e-01 /
CHEB / 3.3133000e+00 1.9353000e+00 1.9688000e-01 /
CHEB / -2.2039000e+00 4.4163000e-01 1.6462000e-01 /
CHEB / -1.4062000e+00 -1.3639000e-01 4.3659000e-02 /
CHEB / -7.1461000e-01 -1.9972000e-01 -2.2205000e-02 /

C3H6+CH2OH(+m)=C4H9O-5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -15.828385675153093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3473000e+00 1.6966000e+00 -3.3324000e-01 /
CHEB / -1.0956000e+00 1.2000000e+00 1.9051000e-01 /
CHEB / -3.1751000e+00 8.0530000e-02 5.4370000e-02 /
CHEB / -1.5065000e+00 -1.8682000e-01 4.1558000e-03 /
CHEB / -5.3877000e-01 -1.2012000e-01 -1.1438000e-02 /
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C3H6+CH2OH(+m)=C4H9O-4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -25.5273818688279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9712000e+00 -2.5082000e-01 -2.3984000e-01 /
CHEB / 1.6443000e+00 2.1870000e+00 -5.5783000e-02 /
CHEB / -2.3661000e+00 6.3970000e-01 1.5682000e-01 /
CHEB / -1.6024000e+00 -1.0613000e-01 8.7480000e-02 /
CHEB / -8.1280000e-01 -2.3745000e-01 -1.3353000e-02 /

C3H6+CH2OH(+m)=C4H9O-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H2_Cd/H/Nd     C_rad/H2/O         deltaHrxn(T=298K) = -
22.097899574448476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1872000e+00 5.8936000e-01 -5.6668000e-02 /
CHEB / -3.4786000e-01 9.0200000e-01 -3.6634000e-02 /
CHEB / -1.9428000e+00 4.1061000e-01 4.5340000e-02 /
CHEB / -1.2327000e+00 4.4044000e-02 5.2515000e-02 /
CHEB / -6.8815000e-01 -1.0961000e-01 1.4577000e-02 /

C3H6+CH2OH(+m)=C4H7-14+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -11.968951236176565
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8952000e+00 -5.2462000e-01 -2.9339000e-01 /
CHEB / 1.6869000e+01 5.7781000e-01 3.0590000e-01 /
CHEB / 1.0105000e-01 6.2719000e-02 5.3860000e-02 /
CHEB / -5.7677000e-02 -9.8835000e-02 -4.6029000e-02 /
CHEB / -2.9092000e-02 -4.0881000e-02 -3.0950000e-02 /

C3H6+CH2OH(+m)=C3H7-1+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -3.4095423784284833
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5026000e+00 -1.0381000e+00 -2.0257000e-01 /
CHEB / 4.9322000e+00 1.1023000e+00 1.4756000e-01 /
CHEB / -6.7921000e-03 1.0988000e-01 8.9778000e-02 /
CHEB / -1.1518000e-01 -1.0144000e-01 1.2612000e-02 /
CHEB / -2.5498000e-02 -7.3272000e-02 -2.7250000e-02 /

C3H6+CH2OH(+m)=C2H5+C2H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -2.0898369601299898
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9059000e+00 -2.0569000e+00 -2.4096000e-01 /
CHEB / 6.5854000e+00 2.0632000e+00 7.6800000e-02 /
CHEB / -4.2984000e-02 3.6001000e-01 2.1073000e-01 /
CHEB / -3.2732000e-01 -1.9069000e-01 4.7800000e-02 /
CHEB / -1.5157000e-01 -1.6373000e-01 -5.0102000e-02 /
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C4H9-1+O(+m)=C4H9O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -96.55011806919495
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3043000e+00 1.4127000e+01 -9.6152000e-01 /
CHEB / -6.2555000e+00 -4.3616000e-01 1.3183000e+00 /
CHEB / -4.0012000e+00 -1.1049000e+00 7.6679000e-01 /
CHEB / -1.8097000e+00 -7.5663000e-01 9.1798000e-02 /
CHEB / -9.0207000e-01 -1.5344000e-01 -1.1522000e-01 /

C4H9-1+O(+m)=C4H9O-3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -98.78012089513692
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0579000e+01 1.4483000e+01 -9.6268000e-01 /
CHEB / -4.4167000e+00 -8.9009000e-01 1.4697000e+00 /
CHEB / -3.1529000e+00 -1.3139000e+00 8.1628000e-01 /
CHEB / -1.3977000e+00 -8.5594000e-01 1.0449000e-01 /
CHEB / -7.3922000e-01 -1.9705000e-01 -1.1187000e-01 /

C4H9-1+O(+m)=C4H9O-5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1) High-P Limit: Oa_R_Recombination estimate:
(Average:) C_rad/H2/Cs     Oa       deltaHrxn(T=298K) = -
93.7103605508635 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4257000e+01 1.3331000e+01 3.2088000e-01 /
CHEB / -6.8086000e+00 -1.4986000e+00 1.2833000e+00 /
CHEB / -3.9600000e+00 -1.5947000e+00 4.5784000e-01 /
CHEB / -1.3952000e+00 -8.2919000e-01 -2.9191000e-01 /
CHEB / -3.7119000e-01 -1.8826000e-01 -2.7590000e-01 /

C4H9-1+O(+m)=C4H9O-4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -103.4093567445383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9469000e+00 1.4084000e+01 -8.9709000e-01 /
CHEB / -6.3336000e+00 -7.5698000e-01 1.3592000e+00 /
CHEB / -3.6084000e+00 -8.5728000e-01 5.8384000e-01 /
CHEB / -1.7359000e+00 -6.2466000e-01 1.8987000e-01 /
CHEB / -8.7092000e-01 -1.1083000e-01 -1.3921000e-01 /

C4H9-1+O(+m)=C4H9O-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -99.97987445015887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.5999000e+00 1.4891000e+01 -9.5351000e-01 /
CHEB / -3.6953000e+00 -1.2490000e+00 1.3271000e+00 /
CHEB / -2.9100000e+00 -1.3436000e+00 7.5668000e-01 /
CHEB / -1.4071000e+00 -7.4814000e-01 6.2637000e-02 /
CHEB / -8.5336000e-01 -8.7441000e-02 -1.3842000e-01 /
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C4H9-1+O(+m)=C2H4+C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -72.52255952643429
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4028000e+00 3.1805000e-03 4.7185000e-04 /
CHEB / 1.9372000e+00 -4.6214000e-03 -1.1593000e-03 /
CHEB / 4.7480000e-01 2.5367000e-03 2.0557000e-03 /
CHEB / 2.6779000e-01 -1.7158000e-03 -2.0906000e-03 /
CHEB / 1.4742000e-01 4.0796000e-05 1.5205000e-04 /

C4H9-1+O(+m)=C4H8O-enol3+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -64.0937090528221
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6999000e+00 -3.1302000e-03 -3.1149000e-03 /
CHEB / 1.7779000e+00 2.3392000e-03 2.7279000e-03 /
CHEB / 4.6274000e-01 2.7505000e-03 2.0575000e-03 /
CHEB / 2.3708000e-01 -2.0896000e-03 -1.8919000e-03 /
CHEB / 1.2781000e-01 -5.0507000e-04 -3.0305000e-04 /

C4H9-1+O(+m)=C4H7-14+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -89.85092611188696
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7680000e+00 -4.4707000e-02 -3.1293000e-02 /
CHEB / 3.4550000e+00 4.5741000e-02 3.2122000e-02 /
CHEB / 1.0672000e+00 1.1509000e-02 7.8487000e-03 /
CHEB / 4.5777000e-01 -1.2002000e-02 -8.2931000e-03 /
CHEB / 1.9835000e-01 -3.5033000e-03 -2.4216000e-03 /

C4H9-1+O(+m)=CH3+C3H6O-enol2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -73.9630269715911
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2828000e+00 -8.3560000e-04 -6.4606000e-04 /
CHEB / 2.2136000e+00 7.1210000e-04 5.6176000e-04 /
CHEB / 6.4888000e-01 4.0459000e-04 3.0973000e-04 /
CHEB / 2.2114000e-01 -2.2687000e-04 -1.9506000e-04 /
CHEB / 6.4547000e-02 -1.4396000e-04 -1.0291000e-04 /

C4H9-1+O(+m)=C4H8O-enol2+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -65.86354617898667
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1673000e+00 6.0418000e-04 3.1972000e-04 /
CHEB / 2.0331000e+00 -1.1311000e-03 -7.0370000e-04 /
CHEB / 6.0411000e-01 7.1561000e-04 5.7247000e-04 /
CHEB / 2.7075000e-01 -6.6719000e-05 -1.0215000e-04 /
CHEB / 1.1933000e-01 -2.5021000e-04 -1.9868000e-04 /
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C4H9-1+O(+m)=C4H8-1+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -69.71294822083365
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7227000e+00 1.0777000e-05 -5.9037000e-05 /
CHEB / 2.0337000e+00 -9.9492000e-05 -2.8921000e-07 /
CHEB / 5.7793000e-01 1.6523000e-04 1.4417000e-04 /
CHEB / 1.9553000e-01 -7.2555000e-05 -9.1106000e-05 /
CHEB / 5.6482000e-02 -5.2266000e-05 -3.8514000e-05 /

C4H9-1+O(+m)=C4H8O-enol+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -70.42310007270683
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1405000e+00 -2.2541000e-02 -1.7684000e-02 /
CHEB / 2.2499000e+00 3.4069000e-02 2.6785000e-02 /
CHEB / 7.3103000e-01 -1.3260000e-02 -1.0465000e-02 /
CHEB / 2.7931000e-01 7.1855000e-04 5.0588000e-04 /
CHEB / 9.4001000e-02 1.3391000e-03 1.1402000e-03 /

C4H9-1+O(+m)=C3H7-1+CH2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -81.29151725413888
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3014000e+01 -2.2944000e-07 -1.6897000e-07 /
CHEB / -5.2361000e-02 1.0362000e-06 7.3124000e-07 /
CHEB / -3.2855000e-02 9.5395000e-07 6.6695000e-07 /
CHEB / -1.5347000e-02 2.2689000e-07 1.5327000e-07 /
CHEB / -1.6475000e-02 -9.6950000e-08 -6.7525000e-08 /

C4H9-1+O(+m)=nC4H8O+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -77.61255532327604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6130000e+00 -9.3202000e-05 -7.8888000e-05 /
CHEB / 1.1006000e+00 1.1358000e-04 9.9998000e-05 /
CHEB / 3.2326000e-01 -2.9920000e-05 -2.7729000e-05 /
CHEB / 1.1696000e-01 1.7427000e-06 -5.6767000e-07 /
CHEB / 3.4742000e-02 1.2431000e-05 1.0717000e-05 /

C4H9-1+O(+m)=C2H5+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -79.97181183584038
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6621000e+00 -1.4452000e-02 -1.2710000e-02 /
CHEB / 2.1869000e+00 2.3757000e-02 2.0719000e-02 /
CHEB / 6.4087000e-01 -1.2063000e-02 -1.0255000e-02 /
CHEB / 2.4709000e-01 2.0155000e-03 1.5672000e-03 /
CHEB / 9.0789000e-02 1.3656000e-03 1.2038000e-03 /
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C4H9-1+O(+m)=C3H6+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O-1)      deltaHrxn(T=298K) = -77.8819748757104
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6187000e+00 4.1184000e-03 2.8207000e-03 /
CHEB / 9.9563000e-01 -4.0406000e-03 -2.7877000e-03 /
CHEB / 2.1005000e-01 -6.9062000e-04 -4.1181000e-04 /
CHEB / 1.2308000e-01 3.5061000e-04 1.9458000e-04 /
CHEB / 8.4587000e-02 1.9404000e-04 1.1253000e-04 /

!PDepNetwork CH2CH[OH]C2H5 + CH3C[OH]C2H5 + CH3CH[OH]CHCH3 +
CH3CH[OH]CH2CH2 + CH3CH[O]C2H5
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CH[OH]C2H5     -20.29      85.12 28.32 34.19 39.3  43.58 50.27
      55.31 63.42  !MRH
!     CH3CH[OH]CHCH3    -22.93      85.73 29.6  34.49 38.99 42.99 49.61
      54.76 63.12  !MRH
!     CH3CH[O]C2H5      -16.68      81.26 27.15 33.15 38.5  43.06 50.3
      55.76 64.36  !MRH
!     CH3C[OH]C2H5      -28.11      85.48 27.09 32.67 37.82 42.25 49.33
      54.67 63.16  !MRH
!     CH3CH[OH]CH2CH2   -21.44      85.19 28.95 34.38 39.34 43.58 50.3
      55.39 63.54  !MRH
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     MEKenol2          -43.57      82.42 24.3  30.12 35.09 39.31 46.17
      51.2  58.73 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H6O-enol        -34.7 70.85 20.67 24.56 28.02 30.98 35.68 39.25
      45.02
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     MEKenol           -46.68      81.2  24.43 29.77 34.47 38.61 45.55
      50.67 58.38 null
!     sC4H8O            -39.25      81.78 24.22 30.55 35.99 40.19 47.0
      51.9  58.85 null
!     C3H6O             -43.67      73.5  18.92 22.42 25.99 29.23 34.57
      38.63 44.94
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     MEK         -56.88      81.06 24.17 29.7  34.59 38.84 46.03 51.35
      58.84 null
```

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!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C4H9-2            18.01 78.98 21.99 27.3  32.36 36.82 44.06 49.58
      58.28
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4O+C2H5=CH2CH[OH]C2H5      2.4827386e+10      0.24400
1.0487500e+04
!     C4H8-1+OH=CH2CH[OH]C2H5 2.7100000e+12      0.00000
0.0000000e+00
!     MEKenol2+H=CH2CH[OH]C2H5      1.1700000e+13      0.00000
4.7000000e+03
!     CH2CH[OH]C2H5=CH3CH[OH]CHCH3  2.3600000e+10      0.82000
3.5100000e+04
!     CH3+C3H6O-enol=CH3CH[OH]CHCH3 1.3600000e+12      0.00000
1.0100000e+04
!     C4H8-2+OH=CH3CH[OH]CHCH3      2.7100000e+12      0.00000
0.0000000e+00
!     MEKenol+H=CH3CH[OH]CHCH3      1.0000000e+13      0.00000
2.9000000e+03
!     sC4H8O+H=CH3CH[OH]CHCH3 2.0100000e+13      0.00000
2.1000000e+03
!     CH3CH[O]C2H5=CH3CH[OH]CHCH3   9.7200000e+09      1.17000
3.9660000e+04
!     CH3+C3H6O=CH3CH[O]C2H5  3.1600000e+10      0.00000
1.1510000e+04
!     CH3CHO+C2H5=CH3CH[O]C2H5      7.9400000e+10      0.00000
6.7000000e+03
!     MEK+H=CH3CH[O]C2H5      1.0000000e+11      0.00000
1.1900000e+04
!     CH3CH[O]C2H5=CH2CH[OH]C2H5    4.2390000e+09      1.45000
4.2270000e+04
!     CH3CH[O]C2H5=CH3C[OH]C2H5     2.0320555e+08      1.13906
3.4790987e+04
!     MEK+H=CH3C[OH]C2H5      2.3501400e+11      0.30815
4.9629937e+03
!     MEKenol2+H=CH3C[OH]C2H5       4.9400000e+13      0.00000
1.5000000e+03
!     H2CCCH3[OH]+CH3=CH3C[OH]C2H5  3.9900000e+12      0.00000
8.0000000e+03
!     MEKenol+H=CH3C[OH]C2H5  1.0000000e+13      0.00000
2.9000000e+03
!     CH3CH[OH]CH2CH2=CH3C[OH]C2H5  1.7526595e+09      0.97886
3.7375179e+04
!     C2H5O-2+C2H4=CH3CH[OH]CH2CH2  1.7353374e+11      0.00000
1.0733333e+04
!     sC4H8O+H=CH3CH[OH]CH2CH2      1.1800000e+13      0.00000
3.8000000e+03
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!     C4H7-14+H2O=CH3CH[OH]CH2CH2   6.5200000e+01      2.92000
5.0700000e+04
!     CH3CH[OH]CH2CH2=CH3CH[OH]CHCH3      3.8760000e+10      0.89000
3.5800000e+04
!     CH2CH[OH]C2H5=CH3CH[OH]CH2CH2 2.2860000e+10      0.35000
1.9760000e+04
!     CH3CH[O]C2H5=CH3CH[OH]CH2CH2  9.0000000e+11      0.00000
2.9400000e+04
!     CH2CH[OH]C2H5=CH3C[OH]C2H5    6.2339791e+09      0.93630
3.7689907e+04
!     CH3CH[OH]CHCH3=CH3C[OH]C2H5   6.2339791e+09      0.93630
3.7689907e+04
!     C4H9-2+O=CH3CH[O]C2H5   1.0000000e+13      0.00000
0.0000000e+00

CH2CH[OH]C2H5(+m)=CH3CH[OH]CHCH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration
exact:  Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.639986649937452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3482000e+00 7.6669000e-01 -6.0002000e-02 /
CHEB / 3.8437000e+00 1.3656000e+00 -1.1368000e-01 /
CHEB / -5.6224000e+00 1.3063000e-01 9.3089000e-02 /
CHEB / -2.9892000e+00 -4.9237000e-01 4.7301000e-02 /
CHEB / -1.0981000e+00 -4.7728000e-01 -3.6137000e-02 /

CH2CH[OH]C2H5(+m)=CH3C[OH]C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_2H     Cs_H_out
      deltaHrxn(T=298K) = -7.819056629276901 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9942000e+00 1.7376000e+00 -2.6630000e-01 /
CHEB / 3.1623000e+00 1.6925000e+00 1.7656000e-03 /
CHEB / -6.2059000e+00 -1.8379000e-02 1.2336000e-01 /
CHEB / -3.1254000e+00 -5.7506000e-01 5.6762000e-03 /
CHEB / -1.0487000e+00 -4.5649000e-01 -5.4177000e-02 /

CH2CH[OH]C2H5(+m)=CH3CH[OH]CH2CH2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration
estimate: (Average:) R4H_SSS     C_rad_out_2H     Cs_H_out_2H
      deltaHrxn(T=298K) = -1.1500069347514028 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4112000e+00 6.1972000e-01 -2.6530000e-02 /
CHEB / -1.8927000e+00 8.3632000e-01 -1.4848000e-02 /
CHEB / -5.9388000e+00 1.5290000e-02 2.8313000e-02 /
CHEB / -3.0921000e+00 -5.3541000e-01 6.0793000e-03 /
CHEB / -9.9444000e-01 -5.0673000e-01 -4.0918000e-02 /

CH3CH[OH]CHCH3(+m)=CH3C[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_H/NonDeC     Cs_H_out
      deltaHrxn(T=298K) = -5.179069979339449 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -7.3660000e+00 1.4828000e+00 -2.7199000e-01 /
CHEB / 5.7867000e+00 1.4997000e+00 -2.3552000e-02 /
CHEB / -4.7828000e+00 1.5508000e-01 1.1910000e-01 /
CHEB / -2.6673000e+00 -3.9376000e-01 3.9648000e-02 /
CHEB / -1.1408000e+00 -3.7171000e-01 -3.6010000e-02 /

CH3CH[O]C2H5(+m)=CH2CH[OH]C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     Cs_H_out_2H
      deltaHrxn(T=298K) = -3.609799878756032 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4827000e+01 2.7646000e+00 4.4857000e-01 /
CHEB / 3.3135000e+00 8.2913000e-01 -1.4953000e-01 /
CHEB / -4.5050000e+00 -2.0784000e-01 -5.3720000e-02 /
CHEB / -2.4327000e+00 -5.5882000e-01 -5.1647000e-04 /
CHEB / -9.5620000e-01 -4.1672000e-01 -8.1293000e-03 /

CH3CH[O]C2H5(+m)=CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -6.249786528693484 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7528000e+01 3.1796000e+00 4.7972000e-01 /
CHEB / 8.2937000e+00 1.2046000e+00 -1.5250000e-01 /
CHEB / -3.0468000e+00 -1.3680000e-01 -9.9302000e-03 /
CHEB / -2.1699000e+00 -4.3808000e-01 9.5014000e-02 /
CHEB / -1.1590000e+00 -3.2167000e-01 6.6399000e-02 /

CH3CH[O]C2H5(+m)=CH3C[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    O_rad_out     Cs_H_out
      deltaHrxn(T=298K) = -11.428856508032933 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7637000e+01 4.8205000e+00 4.0634000e-01 /
CHEB / 6.2463000e+00 6.6862000e-01 -2.7322000e-01 /
CHEB / -3.5438000e+00 -2.2264000e-01 -1.3670000e-01 /
CHEB / -1.8581000e+00 -2.9674000e-01 6.5721000e-03 /
CHEB / -8.2326000e-01 -1.5972000e-01 4.6411000e-02 /

CH3CH[O]C2H5(+m)=CH3CH[OH]CH2CH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration
exact:  R4H_SSS     O_rad_out     Cs_H_out_2H         deltaHrxn(T=298K)
= -4.759806813507435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2670000e+01 4.1602000e+00 4.4911000e-01 /
CHEB / 3.4061000e+00 -8.5205000e-03 -1.3398000e-01 /
CHEB / -4.1078000e+00 -3.4652000e-01 -8.0238000e-02 /
CHEB / -2.1137000e+00 -2.7056000e-01 -1.7003000e-02 /
CHEB / -8.4378000e-01 -1.2198000e-01 1.1938000e-02 /

CH3CH[OH]CH2CH2(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration
estimate: (Average:) Others-R2H_S    C_rad_out_2H
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Cs_H_out_H/(NonDeC/Cs)        deltaHrxn(T=298K) = -1.489979715186049
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8868000e+00 1.1299000e+00 -1.6507000e-01 /
CHEB / 5.0962000e+00 1.1719000e+00 4.1549000e-02 /
CHEB / -5.0947000e+00 1.4376000e-01 1.0080000e-01 /
CHEB / -2.9219000e+00 -4.0214000e-01 3.9790000e-02 /
CHEB / -1.2230000e+00 -4.3100000e-01 -2.6721000e-02 /

CH3CH[OH]CH2CH2(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: intra_H_migration
estimate: (Average:) Others-R3H_SS    C_rad_out_2H     Cs_H_out
      deltaHrxn(T=298K) = -6.669049694525498 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7430000e+00 1.8817000e+00 -3.8387000e-01 /
CHEB / 4.5386000e+00 1.5262000e+00 8.2842000e-02 /
CHEB / -5.6258000e+00 9.0838000e-02 1.3039000e-01 /
CHEB / -3.0757000e+00 -4.9490000e-01 2.1747000e-02 /
CHEB / -1.2001000e+00 -4.5172000e-01 -4.5059000e-02 /

C2H4O+C2H5(+m)=CH2CH[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     C_rad/H2/Cs
      deltaHrxn(T=298K) = -20.598100018939107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1661000e+00 8.7373000e-01 -3.8277000e-02 /
CHEB / -2.8941000e+00 1.2201000e+00 1.4773000e-02 /
CHEB / -4.3153000e+00 3.3842000e-01 6.6489000e-02 /
CHEB / -2.1785000e+00 -1.8773000e-01 1.7947000e-02 /
CHEB / -7.3158000e-01 -2.3347000e-01 -3.0921000e-02 /

C2H4O+C2H5(+m)=CH3CH[OH]CHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
23.23808666887656 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5747000e-01 -6.1607000e-02 -2.1674000e-01 /
CHEB / 3.0142000e+00 2.3556000e+00 -1.2336000e-02 /
CHEB / -2.8379000e+00 5.0631000e-01 1.6437000e-01 /
CHEB / -1.8766000e+00 -2.0175000e-01 5.5105000e-02 /
CHEB / -9.2065000e-01 -2.5735000e-01 -2.0819000e-02 /

C2H4O+C2H5(+m)=CH3CH[O]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
16.988300140183075 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2178000e+01 1.7518000e+00 4.0666000e-01 /
CHEB / 4.3923000e+00 2.0960000e+00 -1.6114000e-01 /
CHEB / -1.7648000e+00 2.6479000e-01 4.4501000e-02 /
CHEB / -1.5748000e+00 -3.6290000e-01 5.9210000e-02 /
CHEB / -9.4611000e-01 -3.1133000e-01 7.9994000e-03 /
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C2H4O+C2H5(+m)=CH3C[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
28.417156648216007 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7768000e+00 1.0429000e+00 -4.2397000e-01 /
CHEB / 2.0039000e+00 2.5464000e+00 1.3283000e-01 /
CHEB / -3.4225000e+00 3.0665000e-01 1.6348000e-01 /
CHEB / -2.0365000e+00 -2.8349000e-01 1.2996000e-02 /
CHEB / -9.0643000e-01 -2.4503000e-01 -2.7163000e-02 /

C2H4O+C2H5(+m)=CH3CH[OH]CH2CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
21.74810695369051 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4399000e+00 -2.6061000e-01 -1.7187000e-01 /
CHEB / -4.2530000e-01 2.1411000e+00 2.4001000e-02 /
CHEB / -3.7920000e+00 5.2988000e-01 1.3581000e-01 /
CHEB / -2.3201000e+00 -2.8081000e-01 3.6168000e-02 /
CHEB / -9.8237000e-01 -3.5433000e-01 -3.9730000e-02 /

C2H4O+C2H5(+m)=CH3+C3H6O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
8.729359911483499 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3466000e+00 -1.7803000e+00 -2.2132000e-01 /
CHEB / 8.7610000e+00 2.0166000e+00 1.6162000e-01 /
CHEB / 7.2254000e-01 1.2874000e-01 1.3271000e-01 /
CHEB / 1.7908000e-01 -3.0651000e-01 -2.9442000e-02 /
CHEB / 1.0256000e-01 -1.5427000e-01 -4.9268000e-02 /

C2H4O+C2H5(+m)=CH3CHO+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.118728856467786 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2665000e-01 -1.8496000e+00 -2.1481000e-01 /
CHEB / 8.0075000e+00 2.0491000e+00 1.4419000e-01 /
CHEB / 5.1193000e-01 1.8964000e-01 1.3867000e-01 /
CHEB / 9.6282000e-02 -3.0485000e-01 -1.9430000e-02 /
CHEB / 7.8621000e-02 -1.7875000e-01 -4.8459000e-02 /

C2H4O+C2H5(+m)=MEK+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.0898551223335815 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1291000e-01 -1.4689000e+00 -2.6755000e-01 /
CHEB / 8.2077000e+00 1.7382000e+00 2.3528000e-01 /
CHEB / 6.5618000e-02 -1.6864000e-02 1.1214000e-01 /
CHEB / -8.5378000e-02 -2.3086000e-01 -4.6185000e-02 /
CHEB / 7.7826000e-03 -8.5474000e-02 -4.4623000e-02 /
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C2H4O+C2H5(+m)=H2CCCH3[OH]+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.499937284952715 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0610000e-01 -1.4218000e+00 -2.7080000e-01 /
CHEB / 8.2449000e+00 1.7038000e+00 2.4427000e-01 /
CHEB / 7.7598000e-02 -4.7563000e-02 1.0735000e-01 /
CHEB / -8.2603000e-02 -2.2370000e-01 -5.0148000e-02 /
CHEB / 1.0292000e-03 -7.1026000e-02 -4.3621000e-02 /

C2H4O+C2H5(+m)=C4H7-14+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
9.879114276046579 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7673000e+00 -3.7893000e-01 -2.3960000e-01 /
CHEB / 1.5125000e+01 4.4106000e-01 2.7052000e-01 /
CHEB / 1.8774000e-01 1.6136000e-02 2.0000000e-02 /
CHEB / 9.2173000e-03 -7.2171000e-02 -4.2524000e-02 /
CHEB / 5.3162000e-03 -2.8020000e-02 -2.1163000e-02 /

C4H8-1+OH(+m)=CH2CH[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     O_pri_rad      deltaHrxn(T=298K)
= -30.85696363394585 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9739000e+00 8.4953000e-01 -3.4017000e-02 /
CHEB / -6.6205000e+00 1.1971000e+00 1.4923000e-02 /
CHEB / -4.3341000e+00 3.3918000e-01 6.3624000e-02 /
CHEB / -2.1934000e+00 -1.8310000e-01 1.7516000e-02 /
CHEB / -7.4190000e-01 -2.3227000e-01 -3.0204000e-02 /

C4H8-1+OH(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
33.4969502838833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5721000e+00 -9.8295000e-02 -2.0842000e-01 /
CHEB / -6.2155000e-01 2.3435000e+00 -1.6749000e-02 /
CHEB / -2.8741000e+00 5.1022000e-01 1.6285000e-01 /
CHEB / -1.8974000e+00 -2.0114000e-01 5.5693000e-02 /
CHEB / -9.3302000e-01 -2.5879000e-01 -2.0739000e-02 /

C4H8-1+OH(+m)=CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
27.247163755189817 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.4125000e+00 1.7195000e+00 4.1261000e-01 /
CHEB / 7.1744000e-01 2.0764000e+00 -1.6196000e-01 /
CHEB / -1.7957000e+00 2.6910000e-01 4.1225000e-02 /
CHEB / -1.5928000e+00 -3.6086000e-01 5.9439000e-02 /
CHEB / -9.5775000e-01 -3.1235000e-01 8.4480000e-03 /
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C4H8-1+OH(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
38.67602026322275 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9522000e+00 1.0015000e+00 -4.1590000e-01 /
CHEB / -1.6251000e+00 2.5394000e+00 1.2787000e-01 /
CHEB / -3.4621000e+00 3.1117000e-01 1.6315000e-01 /
CHEB / -2.0575000e+00 -2.8339000e-01 1.3420000e-02 /
CHEB / -9.1846000e-01 -2.4656000e-01 -2.7409000e-02 /

C4H8-1+OH(+m)=CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
32.006970568697255 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2169000e+00 -2.9660000e-01 -1.6303000e-01 /
CHEB / -4.1180000e+00 2.1260000e+00 1.9375000e-02 /
CHEB / -3.8151000e+00 5.3344000e-01 1.3330000e-01 /
CHEB / -2.3396000e+00 -2.7927000e-01 3.6771000e-02 /
CHEB / -9.9402000e-01 -3.5547000e-01 -3.9363000e-02 /

!C4H8-1+OH(+m)=C2H4O+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.258863615006742 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 1.0694000e+01 -9.9250000e-01 -8.8354000e-02 /
!CHEB / 1.6776000e+00 1.1133000e+00 4.0302000e-02 /
!CHEB / -2.6077000e-01 1.0744000e-01 9.1966000e-02 /
!CHEB / -2.1703000e-01 -1.9011000e-01 -7.9821000e-03 /
!CHEB / -6.3818000e-02 -1.0852000e-01 -4.6209000e-02 /

C4H8-1+OH(+m)=MEKenol2+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
2.040032638553285 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4743000e+00 -9.6111000e-01 -9.7547000e-02 /
CHEB / 2.5308000e+00 1.0917000e+00 5.1419000e-02 /
CHEB / -9.0065000e-02 8.3230000e-02 9.3314000e-02 /
CHEB / -1.4684000e-01 -1.8382000e-01 -1.2567000e-02 /
CHEB / -3.7387000e-02 -9.6250000e-02 -4.6280000e-02 /

C4H8-1+OH(+m)=CH3+C3H6O-enol(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.019344646371486 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0983000e+00 -1.7893000e+00 -2.3869000e-01 /
CHEB / 4.4845000e+00 1.9958000e+00 1.4293000e-01 /
CHEB / -1.1176000e-01 1.1428000e-01 1.6593000e-01 /
CHEB / -2.3930000e-01 -2.4422000e-01 -9.7131000e-03 /
CHEB / -7.9572000e-02 -1.2561000e-01 -4.8860000e-02 /
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C4H8-1+OH(+m)=C4H8-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
2.719803185470054 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0701000e+00 -1.8555000e+00 -2.2677000e-01 /
CHEB / 4.0256000e+00 2.0402000e+00 1.2203000e-01 /
CHEB / -2.2192000e-01 1.5412000e-01 1.6962000e-01 /
CHEB / -2.8566000e-01 -2.4656000e-01 -1.1749000e-03 /
CHEB / -9.5814000e-02 -1.3905000e-01 -4.7069000e-02 /

C4H8-1+OH(+m)=MEKenol+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.149772698791722 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5239000e+00 -1.8535000e+00 -2.2621000e-01 /
CHEB / 4.4916000e+00 2.0396000e+00 1.2224000e-01 /
CHEB / -9.3979000e-02 1.5215000e-01 1.6876000e-01 /
CHEB / -2.3675000e-01 -2.4684000e-01 -1.5536000e-03 /
CHEB / -7.4112000e-02 -1.3841000e-01 -4.6826000e-02 /

C4H8-1+OH(+m)=CH3+C3H6O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.988223526490245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3535000e+00 -1.7975000e+00 -2.1803000e-01 /
CHEB / 5.0864000e+00 2.0292000e+00 1.5634000e-01 /
CHEB / 6.7176000e-01 1.3975000e-01 1.3373000e-01 /
CHEB / 1.5342000e-01 -3.0883000e-01 -2.7684000e-02 /
CHEB / 9.1195000e-02 -1.5948000e-01 -4.9230000e-02 /

C4H8-1+OH(+m)=CH3CHO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
20.377592471474532 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2323000e+00 -1.8675000e+00 -2.1119000e-01 /
CHEB / 4.3301000e+00 2.0608000e+00 1.3865000e-01 /
CHEB / 4.6050000e-01 2.0194000e-01 1.3930000e-01 /
CHEB / 6.9205000e-02 -3.0600000e-01 -1.7462000e-02 /
CHEB / 6.6418000e-02 -1.8395000e-01 -4.8161000e-02 /

C4H8-1+OH(+m)=MEK+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -15.348718737340327 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2767000e+00 -1.4856000e+00 -2.6495000e-01 /
CHEB / 4.5493000e+00 1.7532000e+00 2.3066000e-01 /
CHEB / 1.2557000e-02 -9.6479000e-03 1.1381000e-01 /
CHEB / -1.1068000e-01 -2.3387000e-01 -4.5025000e-02 /
CHEB / -4.6687000e-03 -8.9283000e-02 -4.4972000e-02 /

C4H8-1+OH(+m)=H2CCCH3[OH]+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
14.758800899959454 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5918000e+00 -1.4376000e+00 -2.6846000e-01 /
CHEB / 4.5878000e+00 1.7186000e+00 2.4004000e-01 /
CHEB / 2.5488000e-02 -4.1378000e-02 1.0914000e-01 /
CHEB / -1.0704000e-01 -2.2707000e-01 -4.9203000e-02 /
CHEB / -1.0994000e-02 -7.4523000e-02 -4.4170000e-02 /

C4H8-1+OH(+m)=C2H5O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
9.938729814415423 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2522000e+00 -1.8853000e+00 -2.3707000e-01 /
CHEB / 2.1461000e+00 2.0405000e+00 1.3257000e-01 /
CHEB / -5.3074000e-01 2.3451000e-01 1.7523000e-01 /
CHEB / -4.4723000e-01 -2.7439000e-01 4.2159000e-04 /
CHEB / -1.6974000e-01 -1.9194000e-01 -6.0251000e-02 /

!C4H8-1+OH(+m)=C4H7-14+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
20.137977891053318 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / -2.1310000e+00 -3.7571000e-01 -2.3919000e-01 /
!CHEB / 1.1512000e+01 4.3850000e-01 2.7064000e-01 /
!CHEB / 1.3735000e-01 1.6034000e-02 2.0095000e-02 /
!CHEB / -1.4011000e-02 -7.2969000e-02 -4.3188000e-02 /
!CHEB / -6.6451000e-03 -2.8757000e-02 -2.1738000e-02 /

MEKenol2+H(+m)=CH2CH[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/Nd2_Cd/H2     H_rad      deltaHrxn(T=298K) = -
28.816930995392564 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3780000e+00 9.5478000e-01 -5.3862000e-02 /
CHEB / -5.0512000e+00 1.2907000e+00 1.4996000e-02 /
CHEB / -4.3835000e+00 3.3406000e-01 7.5490000e-02 /
CHEB / -2.1953000e+00 -2.0084000e-01 1.8453000e-02 /
CHEB / -7.3207000e-01 -2.3582000e-01 -3.3338000e-02 /

MEKenol2+H(+m)=CH3CH[OH]CHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
31.456917645330016 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5838000e+00 1.9059000e-01 -2.6865000e-01 /
CHEB / 3.3839000e-01 2.3142000e+00 5.1754000e-02 /
CHEB / -2.8277000e+00 4.7897000e-01 1.5993000e-01 /
CHEB / -1.8581000e+00 -1.8895000e-01 4.7378000e-02 /
CHEB / -8.9153000e-01 -2.2939000e-01 -1.9000000e-02 /

MEKenol2+H(+m)=CH3CH[O]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
25.207131116636532 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -7.8231000e+00 1.9137000e+00 4.2345000e-01 /
CHEB / 2.0748000e+00 2.1037000e+00 -1.9349000e-01 /
CHEB / -1.8034000e+00 2.4985000e-01 5.0912000e-02 /
CHEB / -1.5668000e+00 -3.4118000e-01 7.6454000e-02 /
CHEB / -9.4035000e-01 -3.0405000e-01 8.5815000e-03 /

MEKenol2+H(+m)=CH3C[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H2_Cd/Nd2     H_rad      deltaHrxn(T=298K) = -
36.63598762466947 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0211000e+01 1.0811000e+00 -1.2548000e-01 /
CHEB / -4.9168000e+00 1.4442000e+00 -4.7693000e-02 /
CHEB / -3.5716000e+00 4.2177000e-01 8.7101000e-02 /
CHEB / -1.9625000e+00 -1.2048000e-01 5.2968000e-02 /
CHEB / -8.4645000e-01 -1.9473000e-01 -9.6067000e-03 /

MEKenol2+H(+m)=CH3CH[OH]CH2CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
29.966937930143967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7389000e+00 -1.3819000e-01 -2.0019000e-01 /
CHEB / -2.6705000e+00 2.1906000e+00 4.2996000e-02 /
CHEB / -3.8458000e+00 5.2387000e-01 1.4548000e-01 /
CHEB / -2.3214000e+00 -2.8025000e-01 3.5914000e-02 /
CHEB / -9.7693000e-01 -3.4701000e-01 -3.9481000e-02 /

MEKenol2+H(+m)=C2H4O+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
8.218830976453457 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4870000e+00 -9.5243000e-01 -9.9996000e-02 /
CHEB / 3.1007000e+00 1.0855000e+00 5.4391000e-02 /
CHEB / -1.9291000e-01 7.6484000e-02 9.3536000e-02 /
CHEB / -1.7767000e-01 -1.8166000e-01 -1.3755000e-02 /
CHEB / -4.4716000e-02 -9.2542000e-02 -4.6099000e-02 /

MEKenol2+H(+m)=CH3+C3H6O-enol(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.979312007818201 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1877000e+00 -1.6440000e+00 -2.6233000e-01 /
CHEB / 5.7715000e+00 1.8694000e+00 1.8885000e-01 /
CHEB / 3.2608000e-02 5.7804000e-02 1.4770000e-01 /
CHEB / -1.6708000e-01 -2.3198000e-01 -2.2481000e-02 /
CHEB / -3.7170000e-02 -9.7479000e-02 -4.6948000e-02 /

MEKenol2+H(+m)=C4H8-2+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
0.6797705469167692 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 6.1591000e+00 -1.7005000e+00 -2.5450000e-01 /
CHEB / 5.2982000e+00 1.9092000e+00 1.7290000e-01 /
CHEB / -7.1417000e-02 9.1616000e-02 1.5227000e-01 /
CHEB / -2.0945000e-01 -2.3658000e-01 -1.5263000e-02 /
CHEB / -5.0384000e-02 -1.0937000e-01 -4.6409000e-02 /

MEKenol2+H(+m)=MEKenol+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
3.109740060238437 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7096000e+00 -8.8979000e-01 -1.2703000e-01 /
CHEB / 2.4686000e+00 1.0331000e+00 7.7103000e-02 /
CHEB / 1.0702000e-02 2.4871000e-02 1.0099000e-01 /
CHEB / -8.2129000e-02 -1.5737000e-01 -1.7913000e-02 /
CHEB / 1.4909000e-05 -5.2520000e-02 -4.0700000e-02 /

MEKenol2+H(+m)=CH3+C3H6O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
16.94819088793696 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3224000e+00 -1.5179000e+00 -1.2129000e-01 /
CHEB / 6.3336000e+00 1.7249000e+00 4.3894000e-02 /
CHEB / 7.5177000e-01 9.4930000e-02 1.3095000e-01 /
CHEB / 2.2259000e-01 -2.4782000e-01 -7.3597000e-03 /
CHEB / 1.0573000e-01 -1.3458000e-01 -4.8443000e-02 /

MEKenol2+H(+m)=CH3CHO+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.337559832921247 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1805000e+00 -1.5791000e+00 -1.1250000e-01 /
CHEB / 5.5891000e+00 1.7595000e+00 2.6952000e-02 /
CHEB / 5.3686000e-01 1.4039000e-01 1.3190000e-01 /
CHEB / 1.4759000e-01 -2.4506000e-01 4.1051000e-03 /
CHEB / 8.6510000e-02 -1.5515000e-01 -4.6241000e-02 /

MEKenol2+H(+m)=MEK+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
13.308686098787042 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1150000e+01 -9.9586000e-01 -1.0496000e-01 /
CHEB / 1.3132000e+00 1.0977000e+00 3.8612000e-02 /
CHEB / -1.8519000e-01 1.0984000e-01 1.0554000e-01 /
CHEB / -1.4272000e-01 -1.7148000e-01 4.5318000e-03 /
CHEB / -1.3044000e-02 -8.8387000e-02 -4.1195000e-02 /

MEKenol2+H(+m)=H2CCCH3[OH]+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
12.718768261406169 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2227000e+01 -9.4909000e-01 -1.1392000e-01 /
CHEB / 1.5899000e+00 1.0740000e+00 5.4561000e-02 /
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CHEB / -1.4740000e-01 6.6608000e-02 1.0490000e-01 /
CHEB / -1.3739000e-01 -1.6756000e-01 -6.5153000e-03 /
CHEB / -1.7335000e-02 -6.9738000e-02 -4.2136000e-02 /

MEKenol2+H(+m)=C2H5O-2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.898697175862138 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0903000e+00 -1.8112000e+00 -2.5465000e-01 /
CHEB / 3.5915000e+00 1.9858000e+00 1.5792000e-01 /
CHEB / -3.9456000e-01 1.9090000e-01 1.7351000e-01 /
CHEB / -3.4443000e-01 -2.6682000e-01 -8.1346000e-03 /
CHEB / -1.0398000e-01 -1.7239000e-01 -6.1741000e-02 /

MEKenol2+H(+m)=C4H7-14+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.097945252500033 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9892000e+00 -3.8776000e-01 -2.4057000e-01 /
CHEB / 1.2727000e+01 4.4843000e-01 2.7017000e-01 /
CHEB / 2.8921000e-01 1.5836000e-02 1.9434000e-02 /
CHEB / 7.3003000e-02 -7.0140000e-02 -4.0784000e-02 /
CHEB / 4.7447000e-02 -2.5879000e-02 -1.9511000e-02 /

CH3+C3H6O-enol(+m)=CH2CH[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
20.837618987574363 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2791000e-01 -2.3674000e-01 -1.7501000e-01 /
CHEB / 7.1818000e-01 2.3137000e+00 -2.6672000e-02 /
CHEB / -4.0168000e+00 4.4309000e-01 1.5957000e-01 /
CHEB / -2.2012000e+00 -3.1651000e-01 4.3468000e-02 /
CHEB / -7.7228000e-01 -3.2689000e-01 -3.7066000e-02 /

CH3+C3H6O-enol(+m)=CH3CH[OH]CHCH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit:
R_Addition_MultipleBond estimate: (Average:) C_methyl
Cd/H/Nd_Cd/H/Nd         deltaHrxn(T=298K) = -23.477605637511815 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7802000e+00 7.5799000e-01 -6.3806000e-02 /
CHEB / -7.2901000e-01 1.1368000e+00 -3.7957000e-02 /
CHEB / -2.9440000e+00 4.5012000e-01 5.9686000e-02 /
CHEB / -1.7398000e+00 -2.1812000e-02 5.8364000e-02 /
CHEB / -8.4076000e-01 -1.6026000e-01 7.2636000e-03 /

CH3+C3H6O-enol(+m)=CH3CH[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
17.22781910881833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3862000e+01 2.0859000e+00 4.0814000e-01 /
CHEB / 6.4394000e+00 2.0871000e+00 -1.6512000e-01 /
CHEB / -1.4280000e+00 1.7919000e-01 5.8343000e-02 /
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CHEB / -1.4134000e+00 -2.9514000e-01 1.0358000e-01 /
CHEB / -8.8432000e-01 -2.6805000e-01 2.2627000e-02 /

CH3+C3H6O-enol(+m)=CH3C[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
28.656675616851263 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4030000e-01 6.4880000e-01 -3.8123000e-01 /
CHEB / 1.4886000e+00 2.5907000e+00 6.8330000e-02 /
CHEB / -3.3482000e+00 4.6023000e-01 1.8786000e-01 /
CHEB / -1.9944000e+00 -2.3531000e-01 4.1916000e-02 /
CHEB / -8.7157000e-01 -2.4234000e-01 -2.9158000e-02 /

CH3+C3H6O-enol(+m)=CH3CH[OH]CH2CH2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
21.987625922325766 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3374000e-01 5.9173000e-02 -2.4487000e-01 /
CHEB / 1.7816000e+00 2.1390000e+00 1.0565000e-01 /
CHEB / -3.4843000e+00 4.7340000e-01 1.6120000e-01 /
CHEB / -2.1779000e+00 -2.4385000e-01 4.7399000e-02 /
CHEB / -9.2019000e-01 -3.0800000e-01 -2.3574000e-02 /

CH3+C3H6O-enol(+m)=C2H4O+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
0.2395189686352559 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2891000e+00 -1.7715000e+00 -2.4234000e-01 /
CHEB / 7.9283000e+00 1.9816000e+00 1.4880000e-01 /
CHEB / -9.0352000e-02 1.0509000e-01 1.6478000e-01 /
CHEB / -2.0878000e-01 -2.4204000e-01 -1.1639000e-02 /
CHEB / -6.4400000e-02 -1.2155000e-01 -4.8982000e-02 /

CH3+C3H6O-enol(+m)=CH3+C3H6O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
8.968878880118758 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6642000e+00 -8.6119000e-01 -1.3134000e-01 /
CHEB / 9.9061000e+00 1.0041000e+00 7.0348000e-02 /
CHEB / 5.5175000e-01 -1.6329000e-02 1.1482000e-01 /
CHEB / 8.7766000e-02 -9.8187000e-02 -2.2334000e-02 /
CHEB / 3.1655000e-02 -5.2065000e-02 -3.2435000e-02 /

CH3+C3H6O-enol(+m)=CH3CHO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.358247825103046 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2362000e-01 -9.1812000e-01 -1.1896000e-01 /
CHEB / 9.2258000e+00 1.0567000e+00 4.6566000e-02 /
CHEB / 3.5899000e-01 -3.9430000e-03 1.2336000e-01 /
CHEB / 2.3338000e-02 -9.6415000e-02 -1.5084000e-02 /
CHEB / 1.0737000e-02 -5.9472000e-02 -3.3036000e-02 /
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CH3+C3H6O-enol(+m)=MEK+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.329374090968841 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3391000e+00 -1.6578000e+00 -2.7552000e-01 /
CHEB / 7.6155000e+00 1.8757000e+00 1.9863000e-01 /
CHEB / 4.2568000e-02 7.0243000e-02 1.5623000e-01 /
CHEB / -1.3169000e-01 -2.3523000e-01 -2.4833000e-02 /
CHEB / -9.2860000e-03 -9.7920000e-02 -5.0920000e-02 /

CH3+C3H6O-enol(+m)=H2CCCH3[OH]+CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
4.739456253587967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5979000e+00 -1.6005000e+00 -2.7981000e-01 /
CHEB / 7.7132000e+00 1.8404000e+00 2.1212000e-01 /
CHEB / 6.3421000e-02 3.0175000e-02 1.4971000e-01 /
CHEB / -1.2372000e-01 -2.3239000e-01 -3.2351000e-02 /
CHEB / -1.1340000e-02 -8.4039000e-02 -5.0385000e-02 /

CH3+C3H6O-enol(+m)=C2H5O-2+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) =
0.08061483195606378 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5173000e+00 -1.6830000e+00 -2.9259000e-01 /
CHEB / 7.9185000e+00 1.8526000e+00 1.9687000e-01 /
CHEB / -6.2822000e-02 1.2489000e-01 1.7117000e-01 /
CHEB / -2.7599000e-01 -2.1560000e-01 -9.5816000e-03 /
CHEB / -1.2586000e-01 -1.1224000e-01 -5.1741000e-02 /

CH3+C3H6O-enol(+m)=C4H7-14+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.118633244681831 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9209000e+00 -4.1926000e-01 -2.5143000e-01 /
CHEB / 1.6527000e+01 4.8381000e-01 2.8106000e-01 /
CHEB / 5.2065000e-01 1.0148000e-02 1.7427000e-02 /
CHEB / 6.2523000e-02 -6.8811000e-02 -3.9146000e-02 /
CHEB / -1.1312000e-02 -2.0613000e-02 -1.6135000e-02 /

C4H8-2+OH(+m)=CH2CH[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
28.137160448475797 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0045000e+00 -3.7186000e-01 -1.4801000e-01 /
CHEB / -2.0372000e+00 2.2485000e+00 -4.1740000e-02 /
CHEB / -4.0348000e+00 4.5454000e-01 1.5292000e-01 /
CHEB / -2.2280000e+00 -3.0866000e-01 4.6633000e-02 /
CHEB / -7.9002000e-01 -3.2839000e-01 -3.5695000e-02 /
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C4H8-2+OH(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/Nd     O_pri_rad
      deltaHrxn(T=298K) = -30.777147098413245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0410000e+01 6.4244000e-01 -4.0957000e-02 /
CHEB / -3.9976000e+00 1.0046000e+00 -2.8640000e-02 /
CHEB / -2.8652000e+00 4.3575000e-01 4.5764000e-02 /
CHEB / -1.7440000e+00 -4.8687000e-04 5.2873000e-02 /
CHEB / -8.5599000e-01 -1.4929000e-01 1.0867000e-02 /

C4H8-2+OH(+m)=CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
24.52736056971976 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7048000e+00 1.9567000e+00 4.2692000e-01 /
CHEB / 3.6584000e+00 2.0241000e+00 -1.6628000e-01 /
CHEB / -1.4493000e+00 1.7924000e-01 4.3698000e-02 /
CHEB / -1.4354000e+00 -2.8498000e-01 1.0616000e-01 /
CHEB / -8.9808000e-01 -2.6209000e-01 2.8285000e-02 /

C4H8-2+OH(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
35.9562170777527 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6764000e+00 4.7594000e-01 -3.4938000e-01 /
CHEB / -1.2741000e+00 2.5139000e+00 5.3465000e-02 /
CHEB / -3.3650000e+00 4.7814000e-01 1.8195000e-01 /
CHEB / -2.0224000e+00 -2.2691000e-01 4.5374000e-02 /
CHEB / -8.9135000e-01 -2.4400000e-01 -2.8481000e-02 /

C4H8-2+OH(+m)=CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
29.2871673832272 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7966000e+00 -6.9534000e-02 -2.2280000e-01 /
CHEB / -1.0111000e+00 2.0693000e+00 9.5374000e-02 /
CHEB / -3.4971000e+00 4.8211000e-01 1.5525000e-01 /
CHEB / -2.2009000e+00 -2.3458000e-01 4.9277000e-02 /
CHEB / -9.3729000e-01 -3.0780000e-01 -2.2345000e-02 /

C4H8-2+OH(+m)=C2H4O+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.539060429536686 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2466000e+00 -1.8367000e+00 -2.3084000e-01 /
CHEB / 5.0941000e+00 2.0262000e+00 1.2830000e-01 /
CHEB / -1.8140000e-01 1.4376000e-01 1.6880000e-01 /
CHEB / -2.6926000e-01 -2.4494000e-01 -3.2686000e-03 /
CHEB / -9.1511000e-02 -1.3485000e-01 -4.7435000e-02 /
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C4H8-2+OH(+m)=CH3+C3H6O-enol(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.29954146090143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0278000e+01 -1.0971000e+00 -9.0163000e-02 /
CHEB / 2.2742000e+00 1.1114000e+00 6.5181000e-03 /
CHEB / -2.2467000e-01 2.1307000e-01 1.0228000e-01 /
CHEB / -2.5168000e-01 -1.3575000e-01 3.1982000e-02 /
CHEB / -8.4820000e-02 -1.1153000e-01 -2.8166000e-02 /

C4H8-2+OH(+m)=MEKenol+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
2.429969513321666 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9068000e+00 -1.1415000e+00 -7.8009000e-02 /
CHEB / 2.0317000e+00 1.1228000e+00 -7.2481000e-03 /
CHEB / -1.8188000e-01 2.5698000e-01 9.5100000e-02 /
CHEB / -2.5192000e-01 -1.2696000e-01 4.0640000e-02 /
CHEB / -8.0327000e-02 -1.2402000e-01 -2.2439000e-02 /

C4H8-2+OH(+m)=CH3+C3H6O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
16.26842034102019 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2677000e+00 -9.0193000e-01 -1.1992000e-01 /
CHEB / 7.0723000e+00 1.0496000e+00 5.0030000e-02 /
CHEB / 4.6613000e-01 -1.6164000e-02 1.2336000e-01 /
CHEB / 4.1706000e-02 -9.8248000e-02 -1.8784000e-02 /
CHEB / 1.1447000e-02 -5.6926000e-02 -3.3945000e-02 /

C4H8-2+OH(+m)=CH3CHO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
17.657789286004476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0705000e+00 -9.6515000e-01 -1.0553000e-01 /
CHEB / 6.3880000e+00 1.1075000e+00 2.3944000e-02 /
CHEB / 2.6974000e-01 -2.4701000e-03 1.3081000e-01 /
CHEB / -2.4878000e-02 -9.5799000e-02 -9.9886000e-03 /
CHEB / -1.0313000e-02 -6.4595000e-02 -3.4024000e-02 /

C4H8-2+OH(+m)=MEK+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -12.628915551870271 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3712000e+00 -1.7310000e+00 -2.6385000e-01 /
CHEB / 4.7102000e+00 1.9262000e+00 1.7638000e-01 /
CHEB / -5.0029000e-02 1.1358000e-01 1.6197000e-01 /
CHEB / -1.8897000e-01 -2.3969000e-01 -1.5402000e-02 /
CHEB / -3.3540000e-02 -1.1209000e-01 -5.0449000e-02 /

C4H8-2+OH(+m)=H2CCCH3[OH]+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
12.038997714489398 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6085000e+00 -1.6694000e+00 -2.6946000e-01 /
CHEB / 4.8171000e+00 1.8924000e+00 1.9132000e-01 /
CHEB / -2.5338000e-02 6.7361000e-02 1.5669000e-01 /
CHEB / -1.7768000e-01 -2.3950000e-01 -2.4033000e-02 /
CHEB / -3.3802000e-02 -9.7114000e-02 -5.0956000e-02 /

C4H8-2+OH(+m)=C2H5O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.218926628945367 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4885000e+00 -1.7401000e+00 -2.8361000e-01 /
CHEB / 5.0616000e+00 1.8919000e+00 1.7932000e-01 /
CHEB / -1.4376000e-01 1.5857000e-01 1.7546000e-01 /
CHEB / -3.2958000e-01 -2.1813000e-01 -1.5584000e-03 /
CHEB / -1.5075000e-01 -1.2363000e-01 -5.0673000e-02 /

C4H8-2+OH(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
17.41817470558326 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1799000e+00 -4.0816000e-01 -2.5025000e-01 /
CHEB / 1.3855000e+01 4.7119000e-01 2.7982000e-01 /
CHEB / 4.4516000e-01 1.1560000e-02 1.8277000e-02 /
CHEB / 1.8257000e-02 -6.8599000e-02 -3.9678000e-02 /
CHEB / -3.1638000e-02 -2.1311000e-02 -1.6818000e-02 /

MEKenol+H(+m)=CH2CH[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
25.707190935154127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3137000e+00 -3.7007000e-01 -1.4748000e-01 /
CHEB / -9.8706000e-01 2.2493000e+00 -4.1214000e-02 /
CHEB / -4.0261000e+00 4.5354000e-01 1.5252000e-01 /
CHEB / -2.2209000e+00 -3.0888000e-01 4.6308000e-02 /
CHEB / -7.8173000e-01 -3.2777000e-01 -3.5504000e-02 /

MEKenol+H(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/Nd2_Cd/H/Nd     H_rad         deltaHrxn(T=298K)
= -28.34717758509158 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7180000e+00 6.4253000e-01 -4.0928000e-02 /
CHEB / -2.9479000e+00 1.0048000e+00 -2.8585000e-02 /
CHEB / -2.8559000e+00 4.3588000e-01 4.5812000e-02 /
CHEB / -1.7368000e+00 -3.8359000e-04 5.2909000e-02 /
CHEB / -8.4809000e-01 -1.4922000e-01 1.0892000e-02 /

MEKenol+H(+m)=CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
22.097391056398095 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -1.0087000e+01 2.3955000e+00 5.9260000e-01 /
CHEB / 4.2771000e+00 1.4283000e+00 -3.6692000e-01 /
CHEB / -1.3404000e+00 2.9247000e-01 4.2225000e-02 /
CHEB / -1.3783000e+00 -2.0392000e-01 1.4923000e-01 /
CHEB / -9.1099000e-01 -2.8274000e-01 3.7809000e-02 /

MEKenol+H(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/Nd2     H_rad         deltaHrxn(T=298K)
= -33.52624756443103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8927000e+00 9.9865000e-01 -1.0438000e-01 /
CHEB / -4.2110000e+00 1.3823000e+00 -4.8010000e-02 /
CHEB / -3.5360000e+00 4.2818000e-01 7.8474000e-02 /
CHEB / -1.9566000e+00 -1.0866000e-01 5.3164000e-02 /
CHEB / -8.4915000e-01 -1.9180000e-01 -7.3050000e-03 /

MEKenol+H(+m)=CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
26.85719786990553 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1051000e+00 -6.8831000e-02 -2.2267000e-01 /
CHEB / 3.9126000e-02 2.0700000e+00 9.5606000e-02 /
CHEB / -3.4877000e+00 4.8217000e-01 1.5528000e-01 /
CHEB / -2.1936000e+00 -2.3455000e-01 4.9237000e-02 /
CHEB / -9.2931000e-01 -3.0766000e-01 -2.2321000e-02 /

MEKenol+H(+m)=C2H4O+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.10909091621502 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5626000e+00 -1.8347000e+00 -2.3028000e-01 /
CHEB / 6.1553000e+00 2.0256000e+00 1.2851000e-01 /
CHEB / -1.6361000e-01 1.4180000e-01 1.6794000e-01 /
CHEB / -2.5498000e-01 -2.4521000e-01 -3.6415000e-03 /
CHEB / -7.8434000e-02 -1.3421000e-01 -4.7189000e-02 /

MEKenol+H(+m)=CH3+C3H6O-enol(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.8695719475797645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5866000e+00 -1.0971000e+00 -9.0163000e-02 /
CHEB / 3.3257000e+00 1.1114000e+00 6.5182000e-03 /
CHEB / -2.1380000e-01 2.1307000e-01 1.0228000e-01 /
CHEB / -2.4314000e-01 -1.3575000e-01 3.1982000e-02 /
CHEB / -7.5930000e-02 -1.1153000e-01 -2.8167000e-02 /

MEKenol+H(+m)=CH3+C3H6O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
13.838450827698523 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.6591000e+00 -8.5227000e-01 -1.3361000e-01 /
CHEB / 8.0041000e+00 9.7156000e-01 7.4880000e-02 /
CHEB / 5.3767000e-01 2.2341000e-02 1.0684000e-01 /
CHEB / 3.4287000e-02 -1.1195000e-01 -1.2741000e-02 /
CHEB / 2.5032000e-02 -5.2406000e-02 -3.4523000e-02 /

MEKenol+H(+m)=CH3CHO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
15.22781977268281 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4776000e+00 -9.0117000e-01 -1.2332000e-01 /
CHEB / 7.2949000e+00 1.0066000e+00 5.5506000e-02 /
CHEB / 3.5252000e-01 4.7687000e-02 1.1100000e-01 /
CHEB / -3.4929000e-02 -1.1322000e-01 -3.4601000e-03 /
CHEB / 2.8434000e-03 -5.9616000e-02 -3.4218000e-02 /

MEKenol+H(+m)=MEK+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -10.198946038548605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6692000e+00 -1.0264000e+00 -9.5822000e-02 /
CHEB / 2.0106000e+00 1.1155000e+00 2.6249000e-02 /
CHEB / -1.9714000e-01 1.3313000e-01 1.0401000e-01 /
CHEB / -1.5303000e-01 -1.7365000e-01 1.0813000e-02 /
CHEB / -1.4824000e-02 -9.7110000e-02 -3.9597000e-02 /

MEKenol+H(+m)=H2CCCH3[OH]+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
9.609028201167732 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0716000e+01 -9.7633000e-01 -1.0620000e-01 /
CHEB / 2.3170000e+00 1.0929000e+00 4.3073000e-02 /
CHEB / -1.6208000e-01 8.4637000e-02 1.0540000e-01 /
CHEB / -1.4566000e-01 -1.7143000e-01 -1.2195000e-03 /
CHEB / -1.8683000e-02 -7.6722000e-02 -4.1910000e-02 /

MEKenol+H(+m)=C2H5O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.788957115623701 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7990000e+00 -1.7397000e+00 -2.8353000e-01 /
CHEB / 6.1151000e+00 1.8918000e+00 1.7939000e-01 /
CHEB / -1.3162000e-01 1.5815000e-01 1.7531000e-01 /
CHEB / -3.2012000e-01 -2.1821000e-01 -1.6526000e-03 /
CHEB / -1.4126000e-01 -1.2352000e-01 -5.0643000e-02 /

MEKenol+H(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
14.988205192261596 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.8680000e+00 -4.0792000e-01 -2.5008000e-01 /
CHEB / 1.4910000e+01 4.7095000e-01 2.7967000e-01 /
CHEB / 4.5802000e-01 1.1458000e-02 1.8191000e-02 /
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CHEB / 2.8035000e-02 -6.8531000e-02 -3.9641000e-02 /
CHEB / -2.2061000e-02 -2.1262000e-02 -1.6779000e-02 /

sC4H8O+H(+m)=CH2CH[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
33.136538849960345 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0969000e+00 -1.6475000e-02 -2.5181000e-01 /
CHEB / -4.4530000e+00 2.1701000e+00 5.9489000e-02 /
CHEB / -4.1899000e+00 4.7229000e-01 1.5334000e-01 /
CHEB / -2.2448000e+00 -3.0618000e-01 3.3518000e-02 /
CHEB / -7.9036000e-01 -3.3956000e-01 -4.7717000e-02 /

sC4H8O+H(+m)=CH3CH[OH]CHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H2_Cd/H/Nd     H_rad           deltaHrxn(T=298K) = -
35.776525499897794 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0196000e+01 9.1401000e-01 -1.0017000e-01 /
CHEB / -3.7488000e+00 1.2795000e+00 -3.9695000e-02 /
CHEB / -3.0053000e+00 4.5918000e-01 7.8559000e-02 /
CHEB / -1.7588000e+00 -3.9799000e-02 6.2153000e-02 /
CHEB / -8.3261000e-01 -1.6655000e-01 2.8988000e-03 /

sC4H8O+H(+m)=CH3CH[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
29.52673897120431 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0181000e+00 3.0509000e+00 4.6085000e-01 /
CHEB / 5.8744000e-01 1.1748000e+00 -1.6170000e-01 /
CHEB / -1.6469000e+00 1.0266000e-01 -6.5586000e-03 /
CHEB / -1.3722000e+00 -2.0497000e-01 6.9751000e-02 /
CHEB / -8.4640000e-01 -1.8890000e-01 4.8548000e-02 /

sC4H8O+H(+m)=CH3C[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
40.955595479237246 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2565000e+00 8.8829000e-01 -4.2800000e-01 /
CHEB / -1.9415000e+00 2.6728000e+00 9.6071000e-02 /
CHEB / -3.3223000e+00 4.4318000e-01 1.9476000e-01 /
CHEB / -1.9921000e+00 -2.4284000e-01 3.8586000e-02 /
CHEB / -8.6268000e-01 -2.4316000e-01 -2.9447000e-02 /

sC4H8O+H(+m)=CH3CH[OH]CH2CH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H/Nd_Cd/H2     H_rad           deltaHrxn(T=298K) = -
34.28654578471175 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5137000e+00 1.0890000e+00 -1.4789000e-01 /
CHEB / -4.1076000e+00 1.1582000e+00 6.5016000e-02 /
CHEB / -3.7146000e+00 3.7624000e-01 7.6260000e-02 /
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CHEB / -2.1145000e+00 -1.1530000e-01 4.3046000e-02 /
CHEB / -8.8350000e-01 -2.2978000e-01 2.3978000e-03 /

sC4H8O+H(+m)=C2H4O+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
12.538438831021235 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2271000e+00 -1.7341000e+00 -2.7284000e-01 /
CHEB / 3.0335000e+00 1.9232000e+00 1.8588000e-01 /
CHEB / -2.0190000e-01 1.5406000e-01 1.6902000e-01 /
CHEB / -2.4980000e-01 -2.5871000e-01 -1.6575000e-02 /
CHEB / -6.5784000e-02 -1.5547000e-01 -6.2605000e-02 /

sC4H8O+H(+m)=C4H8-1+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
2.279575216014493 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4898000e+00 -1.7485000e+00 -2.7008000e-01 /
CHEB / 2.9063000e+00 1.9347000e+00 1.8147000e-01 /
CHEB / -2.2825000e-01 1.6274000e-01 1.6983000e-01 /
CHEB / -2.6167000e-01 -2.6137000e-01 -1.4903000e-02 /
CHEB / -7.0466000e-02 -1.6002000e-01 -6.2697000e-02 /

sC4H8O+H(+m)=MEKenol2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.319607854567778 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1051000e+00 -1.6857000e+00 -2.8181000e-01 /
CHEB / 3.9043000e+00 1.8839000e+00 2.0094000e-01 /
CHEB / 5.1307000e-02 1.2641000e-01 1.6521000e-01 /
CHEB / -1.2554000e-01 -2.5064000e-01 -2.2182000e-02 /
CHEB / -4.0097000e-03 -1.4108000e-01 -6.1813000e-02 /

sC4H8O+H(+m)=CH3+C3H6O-enol(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
12.29891986238598 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1079000e+01 -1.0024000e+00 -1.1619000e-01 /
CHEB / 2.1129000e+00 1.0662000e+00 4.1638000e-02 /
CHEB / -6.6288000e-02 1.3555000e-01 1.0845000e-01 /
CHEB / -1.6410000e-01 -1.3965000e-01 1.2963000e-02 /
CHEB / -4.3280000e-02 -8.6283000e-02 -3.5279000e-02 /

sC4H8O+H(+m)=C4H8-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.999378401484547 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1149000e+01 -1.0388000e+00 -1.0775000e-01 /
CHEB / 1.5343000e+00 1.0831000e+00 2.8847000e-02 /
CHEB / -1.7011000e-01 1.6673000e-01 1.0721000e-01 /
CHEB / -1.9743000e-01 -1.3853000e-01 2.0854000e-02 /
CHEB / -5.3721000e-02 -9.6922000e-02 -3.2944000e-02 /
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sC4H8O+H(+m)=MEKenol+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0596000e+01 -1.0388000e+00 -1.0775000e-01 /
CHEB / 1.9911000e+00 1.0831000e+00 2.8847000e-02 /
CHEB / -4.8642000e-02 1.6673000e-01 1.0721000e-01 /
CHEB / -1.5393000e-01 -1.3854000e-01 2.0854000e-02 /
CHEB / -3.6005000e-02 -9.6923000e-02 -3.2945000e-02 /

sC4H8O+H(+m)=CH3+C3H6O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
21.267798742504738 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0342000e+00 -8.7815000e-01 -1.5631000e-01 /
CHEB / 4.8259000e+00 9.3963000e-01 1.0071000e-01 /
CHEB / 7.3485000e-01 1.1044000e-01 9.5523000e-02 /
CHEB / 1.5039000e-01 -1.1810000e-01 7.3892000e-04 /
CHEB / 6.2479000e-02 -7.8932000e-02 -3.3050000e-02 /

sC4H8O+H(+m)=CH3CHO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
22.657167687489025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8922000e+00 -9.0854000e-01 -1.5252000e-01 /
CHEB / 4.0726000e+00 9.5372000e-01 9.1962000e-02 /
CHEB / 5.3431000e-01 1.3708000e-01 9.6635000e-02 /
CHEB / 8.7430000e-02 -1.1667000e-01 7.1365000e-03 /
CHEB / 4.2240000e-02 -8.9587000e-02 -3.1392000e-02 /

sC4H8O+H(+m)=MEK+H(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -17.62829395335482 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3827000e+00 -1.5627000e+00 -2.9183000e-01 /
CHEB / 4.3659000e+00 1.7987000e+00 2.2867000e-01 /
CHEB / 1.6517000e-01 2.6249000e-02 1.4653000e-01 /
CHEB / -9.8619000e-02 -2.2490000e-01 -3.4564000e-02 /
CHEB / -5.4293000e-04 -8.2263000e-02 -4.9811000e-02 /

sC4H8O+H(+m)=H2CCCH3[OH]+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
17.038376115973946 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6684000e+00 -1.5120000e+00 -2.9418000e-01 /
CHEB / 4.4509000e+00 1.7638000e+00 2.3952000e-01 /
CHEB / 1.8185000e-01 -6.6870000e-03 1.3910000e-01 /
CHEB / -9.4713000e-02 -2.1968000e-01 -4.0451000e-02 /
CHEB / -4.4558000e-03 -6.9869000e-02 -4.8231000e-02 /
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sC4H8O+H(+m)=C2H5O-2+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
12.218305030429915 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0205000e+01 -9.0358000e-01 -1.5519000e-01 /
CHEB / 2.3936000e+00 9.4730000e-01 9.2350000e-02 /
CHEB / -1.0914000e-01 1.3228000e-01 9.8383000e-02 /
CHEB / -2.2463000e-01 -1.1088000e-01 8.4250000e-03 /
CHEB / -1.0502000e-01 -8.4008000e-02 -3.0476000e-02 /

sC4H8O+H(+m)=C4H7-14+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
22.41755310706781 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7866000e-01 -2.1621000e-01 -1.2917000e-01 /
CHEB / 1.1626000e+01 2.3376000e-01 1.3528000e-01 /
CHEB / 3.8654000e-01 2.5880000e-02 2.0101000e-02 /
CHEB / 5.6360000e-02 -3.4144000e-02 -1.8203000e-02 /
CHEB / 2.5343000e-03 -1.6369000e-02 -1.1441000e-02 /

CH3+C3H6O(+m)=CH2CH[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
11.868740107455604 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8363000e+00 -1.1917000e-01 -1.4980000e-01 /
CHEB / 3.4432000e+00 2.2998000e+00 8.8597000e-02 /
CHEB / -3.6210000e+00 5.8639000e-01 1.6942000e-01 /
CHEB / -2.0713000e+00 -2.4656000e-01 4.5665000e-02 /
CHEB / -7.2858000e-01 -2.9851000e-01 -3.4267000e-02 /

CH3+C3H6O(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
14.508726757393056 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8828000e+00 1.1548000e+00 -8.5357000e-02 /
CHEB / 7.4840000e+00 1.8161000e+00 -8.3592000e-02 /
CHEB / -2.4522000e+00 2.4323000e-01 1.6322000e-01 /
CHEB / -1.5834000e+00 -8.2047000e-02 5.8711000e-02 /
CHEB / -7.7321000e-01 -1.6368000e-01 -1.5478000e-02 /

CH3+C3H6O(+m)=CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_methyl     CO/H/Nd_O           deltaHrxn(T=298K)
= -8.258940228699572 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1405000e+00 3.0140000e+00 1.1717000e-01 /
CHEB / -9.8776000e-01 6.9408000e-02 -3.8785000e-02 /
CHEB / -2.5374000e+00 -1.1663000e-01 -1.6347000e-02 /
CHEB / -1.1456000e+00 -5.9760000e-02 -1.4764000e-02 /
CHEB / -5.0327000e-01 1.5325000e-03 -6.1741000e-03 /
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CH3+C3H6O(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
19.687796736732505 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.6738000e+00 2.0111000e+00 -3.8378000e-01 /
CHEB / 4.9068000e+00 1.7589000e+00 7.9417000e-02 /
CHEB / -3.0728000e+00 3.4567000e-01 1.5872000e-01 /
CHEB / -1.7324000e+00 -1.7075000e-01 4.8770000e-02 /
CHEB / -7.4385000e-01 -1.9081000e-01 -1.7732000e-02 /

CH3+C3H6O(+m)=CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
13.018747042207007 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2837000e+00 9.5358000e-01 -9.1746000e-02 /
CHEB / 3.5183000e+00 1.1853000e+00 5.0695000e-02 /
CHEB / -3.1442000e+00 4.2258000e-01 8.4890000e-02 /
CHEB / -1.9277000e+00 -6.1716000e-02 4.7165000e-02 /
CHEB / -8.2818000e-01 -1.9257000e-01 6.4423000e-03 /

CH3+C3H6O(+m)=CH3CHO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
1.3893689449842874 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9237000e+00 -3.9768000e-03 -3.1238000e-03 /
CHEB / 3.7547000e+00 5.7155000e-03 4.4858000e-03 /
CHEB / -1.9963000e-02 -1.5847000e-03 -1.2385000e-03 /
CHEB / 6.0795000e-03 -5.3500000e-04 -4.2097000e-04 /
CHEB / -2.2542000e-03 3.5803000e-04 2.7720000e-04 /

CH3+C3H6O(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
1.1497543645630728 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5205000e+01 -2.0939000e-01 -1.2772000e-01 /
CHEB / 2.0066000e+01 2.2576000e-01 1.3354000e-01 /
CHEB / 9.4885000e-01 2.6406000e-02 2.0417000e-02 /
CHEB / 3.2632000e-01 -3.3640000e-02 -1.8287000e-02 /
CHEB / 1.2927000e-01 -1.6536000e-02 -1.1654000e-02 /

CH3CHO+C2H5(+m)=CH2CH[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.479371162471317 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6002000e+00 -2.6338000e-01 -1.3183000e-01 /
CHEB / 3.4882000e+00 2.1718000e+00 8.2017000e-02 /
CHEB / -3.6539000e+00 5.8440000e-01 1.6352000e-01 /
CHEB / -2.0864000e+00 -2.3229000e-01 5.0561000e-02 /
CHEB / -7.4207000e-01 -2.9917000e-01 -3.1583000e-02 /
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CH3CHO+C2H5(+m)=CH3CH[OH]CHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
13.119357812408769 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7784000e+00 9.7164000e-01 -5.5899000e-02 /
CHEB / 7.6641000e+00 1.7614000e+00 -9.9322000e-02 /
CHEB / -2.4936000e+00 2.1978000e-01 1.4838000e-01 /
CHEB / -1.6101000e+00 -7.3369000e-02 6.3724000e-02 /
CHEB / -7.8404000e-01 -1.5640000e-01 -1.3101000e-02 /

CH3CHO+C2H5(+m)=CH3CH[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H/Nd_O     C_rad/H2/Cs        deltaHrxn(T=298K)
= -6.869571283715285 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7384000e+00 1.6229000e+00 -9.7309000e-02 /
CHEB / -2.9046000e+00 4.4138000e-01 1.2213000e-01 /
CHEB / -2.6331000e+00 -1.5544000e-02 -1.1335000e-02 /
CHEB / -1.1931000e+00 -5.2418000e-02 -1.4671000e-02 /
CHEB / -5.1639000e-01 -9.1205000e-03 -2.6668000e-03 /

CH3CHO+C2H5(+m)=CH3C[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.298427791748217 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4552000e+00 1.8660000e+00 -3.7704000e-01 /
CHEB / 5.1006000e+00 1.6308000e+00 6.0078000e-02 /
CHEB / -3.1208000e+00 3.3124000e-01 1.4781000e-01 /
CHEB / -1.7574000e+00 -1.6076000e-01 5.0207000e-02 /
CHEB / -7.5788000e-01 -1.8728000e-01 -1.5008000e-02 /

CH3CHO+C2H5(+m)=CH3CH[OH]CH2CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
11.62937809722272 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9822000e+00 8.3640000e-01 -7.8081000e-02 /
CHEB / 3.5094000e+00 1.0503000e+00 4.7719000e-02 /
CHEB / -3.2094000e+00 3.8485000e-01 7.6828000e-02 /
CHEB / -1.9339000e+00 -5.5518000e-02 4.3885000e-02 /
CHEB / -8.2941000e-01 -1.8069000e-01 7.1714000e-03 /

MEK+H(+m)=CH2CH[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
15.508244896605522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3074000e+00 8.2558000e-02 -2.1195000e-01 /
CHEB / 2.3034000e+00 2.1048000e+00 8.8219000e-02 /
CHEB / -4.1330000e+00 2.6663000e-01 1.3037000e-01 /
CHEB / -2.1515000e+00 -3.2444000e-01 -6.0414000e-03 /
CHEB / -7.1004000e-01 -2.7594000e-01 -4.5612000e-02 /
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MEK+H(+m)=CH3CH[OH]CHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.148231546542974 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9838000e-02 -1.7690000e-02 -2.4327000e-01 /
CHEB / 3.8798000e+00 2.1470000e+00 6.0077000e-02 /
CHEB / -2.8579000e+00 4.7591000e-01 1.5961000e-01 /
CHEB / -1.7869000e+00 -1.7187000e-01 4.1479000e-02 /
CHEB / -8.3389000e-01 -2.1528000e-01 -2.9039000e-02 /

MEK+H(+m)=CH3CH[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/Nd2_O     H_rad         deltaHrxn(T=298K) = -
11.89844501784949 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0851000e+00 3.3764000e+00 2.2695000e-01 /
CHEB / -6.6698000e-01 6.5510000e-02 -4.0261000e-02 /
CHEB / -2.4491000e+00 -1.8667000e-01 -1.7462000e-02 /
CHEB / -1.1398000e+00 -5.4793000e-02 -2.0156000e-02 /
CHEB / -5.1864000e-01 3.6592000e-02 -1.5093000e-02 /

MEK+H(+m)=CH3C[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
23.327301525882422 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9915000e+00 5.9011000e-01 -2.6500000e-02 /
CHEB / -2.7410000e+00 9.2665000e-01 -1.8342000e-02 /
CHEB / -3.1810000e+00 3.8771000e-01 3.5245000e-02 /
CHEB / -1.8818000e+00 -3.6773000e-02 4.1129000e-02 /
CHEB / -8.5039000e-01 -1.6299000e-01 6.6771000e-03 /

MEK+H(+m)=CH3CH[OH]CH2CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
16.658251831356925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6829000e+00 2.0366000e-01 -2.8962000e-01 /
CHEB / 3.4112000e+00 1.9617000e+00 1.6366000e-01 /
CHEB / -3.5195000e+00 4.0832000e-01 1.5616000e-01 /
CHEB / -2.1318000e+00 -2.4924000e-01 1.8586000e-02 /
CHEB / -8.8015000e-01 -2.8115000e-01 -2.8010000e-02 /

MEK+H(+m)=CH3+C3H6O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -3.6395047891499175 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9614000e+00 -2.4226000e-03 -1.6832000e-03 /
CHEB / 5.0566000e+00 3.2397000e-03 2.2509000e-03 /
CHEB / 2.3786000e-01 -6.1860000e-04 -4.2965000e-04 /
CHEB / 5.3075000e-02 -3.2111000e-04 -2.2329000e-04 /
CHEB / 1.4689000e-02 7.9280000e-05 5.5156000e-05 /
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MEK+H(+m)=CH3CHO+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.028873734134205 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2787000e+00 -4.1751000e-04 -3.4223000e-04 /
CHEB / 3.8859000e+00 5.7056000e-04 4.6729000e-04 /
CHEB / -3.5190000e-03 -1.0241000e-04 -8.3240000e-05 /
CHEB / 1.0697000e-02 -9.6687000e-05 -7.9752000e-05 /
CHEB / 7.5567000e-03 3.6568000e-05 2.9815000e-05 /

MEK+H(+m)=H2CCCH3[OH]+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) =
0.5899178373808738 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2534000e+00 -1.1099000e+00 -7.2306000e-02 /
CHEB / 4.3199000e+00 1.1472000e+00 -2.2075000e-03 /
CHEB / -3.2588000e-01 2.1349000e-01 9.2909000e-02 /
CHEB / -2.3958000e-01 -1.6931000e-01 2.8696000e-02 /
CHEB / -3.8641000e-02 -1.2583000e-01 -3.1069000e-02 /

MEK+H(+m)=C4H7-14+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.78925915371299 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0821000e+01 -3.1568000e-01 -2.0231000e-01 /
CHEB / 1.8487000e+01 3.7178000e-01 2.3360000e-01 /
CHEB / 5.5443000e-01 -3.6921000e-03 3.2563000e-03 /
CHEB / 1.0647000e-01 -4.9550000e-02 -3.0519000e-02 /
CHEB / 2.2923000e-02 -1.3336000e-02 -1.0176000e-02 /

H2CCCH3[OH]+CH3(+m)=CH2CH[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
16.098162733986396 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5904000e+00 2.1589000e-01 -2.2664000e-01 /
CHEB / 2.0606000e+00 2.1896000e+00 9.6865000e-02 /
CHEB / -4.1301000e+00 2.7032000e-01 1.3189000e-01 /
CHEB / -2.1329000e+00 -3.2745000e-01 -7.5718000e-03 /
CHEB / -6.9856000e-01 -2.7421000e-01 -4.4865000e-02 /

H2CCCH3[OH]+CH3(+m)=CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
18.738149383923847 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6283000e-01 1.2884000e-01 -2.5864000e-01 /
CHEB / 3.6774000e+00 2.2619000e+00 6.8108000e-02 /
CHEB / -2.8619000e+00 4.7723000e-01 1.6465000e-01 /
CHEB / -1.7722000e+00 -1.7856000e-01 3.8343000e-02 /
CHEB / -8.2051000e-01 -2.1349000e-01 -2.9900000e-02 /
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```
H2CCCH3[OH]+CH3(+m)=CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
12.488362855230363 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4510000e+01 3.0208000e+00 5.4854000e-01 /
CHEB / 5.7559000e+00 1.2085000e+00 -1.6835000e-01 /
CHEB / -1.5800000e+00 9.4806000e-02 -7.6477000e-02 /
CHEB / -1.0283000e+00 -1.7939000e-01 5.6374000e-02 /
CHEB / -6.3905000e-01 -1.5941000e-01 7.9125000e-02 /

H2CCCH3[OH]+CH3(+m)=CH3C[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit:
R_Addition_MultipleBond exact:  Cd/H2_Cd/Nd2     C_methyl
      deltaHrxn(T=298K) = -23.917219363263296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6713000e+00 7.6989000e-01 -5.5182000e-02 /
CHEB / -2.0692000e+00 1.1557000e+00 -3.6819000e-02 /
CHEB / -3.3880000e+00 4.2300000e-01 5.2801000e-02 /
CHEB / -1.9067000e+00 -7.2921000e-02 4.9628000e-02 /
CHEB / -8.3781000e-01 -1.8196000e-01 3.3331000e-04 /

H2CCCH3[OH]+CH3(+m)=CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
17.2481696687378 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0059000e+00 3.1353000e-01 -3.0579000e-01 /
CHEB / 3.2205000e+00 2.0812000e+00 1.8086000e-01 /
CHEB / -3.5229000e+00 4.0468000e-01 1.5016000e-01 /
CHEB / -2.1165000e+00 -2.4912000e-01 2.1875000e-02 /
CHEB / -8.7121000e-01 -2.8315000e-01 -2.7662000e-02 /

H2CCCH3[OH]+CH3(+m)=CH3+C3H6O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
4.229422626530791 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7595000e+00 -6.9081000e-01 -1.7861000e-01 /
CHEB / 9.9373000e+00 8.2749000e-01 1.6479000e-01 /
CHEB / 6.2193000e-01 -1.8367000e-02 6.8379000e-02 /
CHEB / 2.4297000e-01 -1.1900000e-01 -3.5868000e-02 /
CHEB / 1.4907000e-01 -3.0675000e-02 -3.0632000e-02 /

H2CCCH3[OH]+CH3(+m)=CH3CHO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.618791571515079 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8865000e-01 -7.2405000e-01 -1.7849000e-01 /
CHEB / 9.1913000e+00 8.4796000e-01 1.5701000e-01 /
CHEB / 4.0230000e-01 6.2294000e-03 7.5565000e-02 /
CHEB / 1.7549000e-01 -1.2175000e-01 -3.0670000e-02 /
CHEB / 1.2929000e-01 -4.0528000e-02 -3.3046000e-02 /
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H2CCCH3[OH]+CH3(+m)=C4H7-14+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.379176991093864 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0641000e+01 -3.3445000e-01 -2.0740000e-01 /
CHEB / 1.8219000e+01 3.9287000e-01 2.3869000e-01 /
CHEB / 6.1720000e-01 -4.6877000e-03 3.1670000e-03 /
CHEB / 1.4968000e-01 -5.0711000e-02 -3.0349000e-02 /
CHEB / 3.9759000e-02 -1.2992000e-02 -9.8108000e-03 /

C2H5O-2+C2H4(+m)=CH2CH[OH]C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
20.91823381953043 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4059000e+00 -3.1440000e-01 -1.7380000e-01 /
CHEB / -1.6885000e+00 2.0749000e+00 1.4665000e-02 /
CHEB / -4.1631000e+00 4.9104000e-01 1.3606000e-01 /
CHEB / -2.2988000e+00 -3.0032000e-01 3.7865000e-02 /
CHEB / -8.3335000e-01 -3.4796000e-01 -4.5124000e-02 /

C2H5O-2+C2H4(+m)=CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
23.558220469467877 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9881000e-01 1.1081000e-01 -2.7633000e-01 /
CHEB / 2.8491000e+00 2.2274000e+00 6.9823000e-02 /
CHEB / -2.7134000e+00 5.0156000e-01 1.8374000e-01 /
CHEB / -1.8521000e+00 -1.8062000e-01 6.2616000e-02 /
CHEB / -9.2158000e-01 -2.5129000e-01 -2.2254000e-02 /

C2H5O-2+C2H4(+m)=CH3CH[O]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
17.308433940774393 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0552000e+01 2.8354000e+00 4.9929000e-01 /
CHEB / 3.1990000e+00 1.0196000e+00 -1.5564000e-01 /
CHEB / -1.6546000e+00 9.4203000e-02 -2.4153000e-02 /
CHEB / -1.3857000e+00 -1.8808000e-01 6.2501000e-02 /
CHEB / -8.7394000e-01 -1.7745000e-01 5.0233000e-02 /

C2H5O-2+C2H4(+m)=CH3C[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
28.73729044880733 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2509000e+00 9.7448000e-01 -4.7775000e-01 /
CHEB / 1.9727000e+00 2.5181000e+00 1.5297000e-01 /
CHEB / -3.2278000e+00 3.9526000e-01 2.0262000e-01 /
CHEB / -2.0094000e+00 -2.5338000e-01 4.3414000e-02 /
CHEB / -9.2244000e-01 -2.5552000e-01 -2.5006000e-02 /

C2H5O-2+C2H4(+m)=CH3CH[OH]CH2CH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit:
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R_Addition_MultipleBond estimate: (Average:) C_rad/H/CsO     Cd/H2_Cd/H2
      deltaHrxn(T=298K) = -22.06824075428183 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0665000e+00 8.3949000e-01 -8.2573000e-02 /
CHEB / -1.6286000e+00 1.0531000e+00 3.3346000e-02 /
CHEB / -3.6674000e+00 3.5104000e-01 7.0965000e-02 /
CHEB / -2.1311000e+00 -1.0010000e-01 3.8865000e-02 /
CHEB / -9.1574000e-01 -2.1578000e-01 2.0403000e-03 /

C2H5O-2+C2H4(+m)=C2H4O+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
0.3201338005913179 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9840000e+00 -1.8681000e+00 -2.4113000e-01 /
CHEB / 5.8533000e+00 2.0284000e+00 1.3834000e-01 /
CHEB / -4.2664000e-01 2.2369000e-01 1.7504000e-01 /
CHEB / -4.1097000e-01 -2.7281000e-01 -1.6176000e-03 /
CHEB / -1.5601000e-01 -1.8716000e-01 -6.0687000e-02 /

C2H5O-2+C2H4(+m)=CH3+C3H6O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
9.04949371207482 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4983000e-01 -9.5703000e-01 -1.3975000e-01 /
CHEB / 7.4399000e+00 9.9361000e-01 7.0655000e-02 /
CHEB / 5.0081000e-01 1.5431000e-01 1.0040000e-01 /
CHEB / 3.1884000e-02 -1.1630000e-01 1.4576000e-02 /
CHEB / 2.4044000e-02 -9.5141000e-02 -2.9058000e-02 /

C2H5O-2+C2H4(+m)=CH3CHO+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.438862657059108 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6670000e+00 -9.9207000e-01 -1.3315000e-01 /
CHEB / 6.6547000e+00 1.0076000e+00 6.0247000e-02 /
CHEB / 2.9713000e-01 1.8602000e-01 9.8894000e-02 /
CHEB / -4.0497000e-02 -1.1226000e-01 2.1082000e-02 /
CHEB / -3.0654000e-03 -1.0722000e-01 -2.5601000e-02 /

C2H5O-2+C2H4(+m)=MEK+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
5.409988922924903 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0321000e-01 -1.5298000e+00 -3.1466000e-01 /
CHEB / 8.1280000e+00 1.7151000e+00 2.5268000e-01 /
CHEB / 1.3558000e-01 7.9662000e-02 1.3886000e-01 /
CHEB / -1.6940000e-01 -2.0362000e-01 -2.5653000e-02 /
CHEB / -6.7902000e-02 -9.9335000e-02 -4.3618000e-02 /

C2H5O-2+C2H4(+m)=H2CCCH3[OH]+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH2CH[OH]C2H5) deltaHrxn(T=298K) = -
4.820071085544029 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1904000e+00 -1.4885000e+00 -3.1586000e-01 /
CHEB / 8.1983000e+00 1.6907000e+00 2.6112000e-01 /
CHEB / 1.4762000e-01 4.8006000e-02 1.3283000e-01 /
CHEB / -1.6255000e-01 -2.0068000e-01 -3.0194000e-02 /
CHEB / -6.7633000e-02 -8.7514000e-02 -4.3757000e-02 /

C2H5O-2+C2H4(+m)=C4H7-14+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.199248076637893 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3874000e+00 -2.0351000e-01 -1.2623000e-01 /
CHEB / 1.4964000e+01 2.2022000e-01 1.3255000e-01 /
CHEB / 2.2036000e-01 2.6254000e-02 2.0442000e-02 /
CHEB / -1.9624000e-02 -3.3861000e-02 -1.8716000e-02 /
CHEB / -3.8152000e-02 -1.6982000e-02 -1.2062000e-02 /

C4H7-14+H2O(+m)=CH2CH[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
10.718985742892531 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8661000e+01 4.8095000e+00 -1.1191000e+00 /
CHEB / 1.1405000e+01 9.2029000e-01 5.9485000e-01 /
CHEB / -4.2921000e+00 7.4940000e-02 2.4542000e-01 /
CHEB / -2.2150000e+00 -3.3809000e-01 1.0914000e-02 /
CHEB / -7.9178000e-01 -2.7965000e-01 -6.1886000e-02 /

C4H7-14+H2O(+m)=CH3CH[OH]CHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
13.358972392829983 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9319000e+01 5.3019000e+00 -1.2299000e+00 /
CHEB / 1.4738000e+01 9.5556000e-01 6.7105000e-01 /
CHEB / -2.7184000e+00 1.0032000e-01 2.6262000e-01 /
CHEB / -1.7128000e+00 -2.2333000e-01 3.3644000e-02 /
CHEB / -8.6289000e-01 -1.9557000e-01 -3.9926000e-02 /

C4H7-14+H2O(+m)=CH3CH[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
7.109185864136499 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2348000e+01 7.2695000e+00 -2.6102000e-01 /
CHEB / 1.7090000e+01 5.7344000e-01 1.4381000e-01 /
CHEB / -1.7370000e+00 -2.4148000e-01 1.6709000e-01 /
CHEB / -1.4368000e+00 -3.2988000e-01 7.3362000e-02 /
CHEB / -8.8778000e-01 -1.9190000e-01 1.6482000e-02 /

C4H7-14+H2O(+m)=CH3C[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
18.538042372169432 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -2.2455000e+01 6.4638000e+00 -1.3198000e+00 /
CHEB / 1.3945000e+01 8.7905000e-01 6.5785000e-01 /
CHEB / -3.0649000e+00 9.9199000e-03 2.4806000e-01 /
CHEB / -1.8704000e+00 -2.2787000e-01 4.3129000e-02 /
CHEB / -8.9039000e-01 -1.8884000e-01 -2.5225000e-02 /

C4H7-14+H2O(+m)=CH3CH[OH]CH2CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: 1,3_Insertion_ROR exact:
Cd/H2_Cd/H/Nd     H_OH        deltaHrxn(T=298K) = -11.868992677643934
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7882000e+01 5.4180000e+00 -9.5841000e-01 /
CHEB / 1.2489000e+01 4.0251000e-01 4.9247000e-01 /
CHEB / -3.8342000e+00 7.7526000e-02 2.1963000e-01 /
CHEB / -2.1809000e+00 -2.3439000e-01 3.9898000e-02 /
CHEB / -9.2313000e-01 -2.3428000e-01 -2.8682000e-02 /

C4H7-14+H2O(+m)=CH3CHO+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
0.23961458042121464 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4606000e+01 -1.9780000e-01 -1.2506000e-01 /
CHEB / 1.9904000e+01 2.1417000e-01 1.3127000e-01 /
CHEB / 7.5465000e-01 2.6061000e-02 2.0634000e-02 /
CHEB / 2.6504000e-01 -3.3628000e-02 -1.8834000e-02 /
CHEB / 1.1397000e-01 -1.7180000e-02 -1.2350000e-02 /

C4H9-2+O(+m)=CH2CH[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
97.93030860396092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0910000e+01 1.3454000e+01 -3.9031000e-01 /
CHEB / -3.6949000e+00 -1.7154000e+00 4.5457000e-01 /
CHEB / -3.7552000e+00 -1.1561000e+00 4.3854000e-01 /
CHEB / -2.1399000e+00 -5.8908000e-01 1.2517000e-01 /
CHEB / -8.9787000e-01 -1.4555000e-01 -6.0821000e-02 /

C4H9-2+O(+m)=CH3CH[OH]CHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
100.57029525389838 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0346000e+01 1.4129000e+01 -3.5708000e-01 /
CHEB / -1.7835000e+00 -1.8303000e+00 4.6316000e-01 /
CHEB / -2.0647000e+00 -1.2090000e+00 3.6300000e-01 /
CHEB / -1.5115000e+00 -4.7372000e-01 1.3574000e-01 /
CHEB / -9.5781000e-01 -2.8518000e-02 -1.6228000e-02 /

C4H9-2+O(+m)=CH3CH[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5) High-P Limit: Oa_R_Recombination
estimate: (Average:) C_rad/H/NonDeC     Oa      deltaHrxn(T=298K) = -
94.32050872520489 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -1.9127000e+01 7.9264000e+00 2.3496000e+00 /
CHEB / -1.9160000e+00 3.0458000e+00 8.9411000e-02 /
CHEB / -2.0715000e+00 1.2075000e-02 -4.0942000e-01 /
CHEB / -1.3602000e+00 -4.3437000e-01 -1.8282000e-01 /
CHEB / -7.8485000e-01 -3.3678000e-01 9.5573000e-03 /

C4H9-2+O(+m)=CH3C[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
105.74936523323782 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4070000e+01 1.5201000e+01 -3.6414000e-01 /
CHEB / -2.0816000e+00 -1.8734000e+00 2.3949000e-01 /
CHEB / -2.1765000e+00 -1.2180000e+00 4.4823000e-01 /
CHEB / -1.8078000e+00 -4.6584000e-01 2.3033000e-01 /
CHEB / -1.0349000e+00 -5.3266000e-02 -4.4897000e-02 /

C4H9-2+O(+m)=CH3CH[OH]CH2CH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
99.08031553871233 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0239000e+01 1.3891000e+01 -3.1740000e-01 /
CHEB / -2.4891000e+00 -2.0451000e+00 4.4301000e-01 /
CHEB / -3.3029000e+00 -1.1570000e+00 4.1770000e-01 /
CHEB / -2.1221000e+00 -5.1226000e-01 1.3936000e-01 /
CHEB / -1.0358000e+00 -1.1178000e-01 -3.5327000e-02 /

C4H9-2+O(+m)=C2H4O+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
77.33220858502182 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3312000e+00 2.7762000e-04 1.9171000e-04 /
CHEB / 2.4263000e+00 -3.4341000e-04 -2.3837000e-04 /
CHEB / 8.0284000e-01 1.5037000e-05 1.3168000e-05 /
CHEB / 2.6391000e-01 5.6005000e-05 3.7119000e-05 /
CHEB / 6.9773000e-02 3.6370000e-06 1.7117000e-06 /

C4H9-2+O(+m)=C4H8-1+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
67.07334497001509 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4979000e+00 4.6423000e-04 3.2455000e-04 /
CHEB / 2.3712000e+00 -5.3357000e-04 -3.7406000e-04 /
CHEB / 7.8475000e-01 -1.7954000e-05 -1.0132000e-05 /
CHEB / 2.5756000e-01 8.4533000e-05 5.7730000e-05 /
CHEB / 6.7642000e-02 1.6435000e-05 1.0744000e-05 /

C4H9-2+O(+m)=MEKenol2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
69.11337760856836 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4994000e+00 -3.8042000e-04 -2.7441000e-04 /
CHEB / 2.9606000e+00 3.6185000e-04 2.6205000e-04 /
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CHEB / 9.6732000e-01 7.6568000e-05 5.6065000e-05 /
CHEB / 3.2730000e-01 -3.2983000e-05 -2.6428000e-05 /
CHEB / 9.6416000e-02 -3.1046000e-05 -2.2673000e-05 /

C4H9-2+O(+m)=CH3+C3H6O-enol(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
77.09268961638656 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3418000e+00 -5.4174000e-04 -4.0166000e-04 /
CHEB / 2.2880000e+00 6.0056000e-04 4.4851000e-04 /
CHEB / 7.4307000e-01 4.0549000e-05 2.6890000e-05 /
CHEB / 2.4647000e-01 -8.8857000e-05 -6.7872000e-05 /
CHEB / 7.0911000e-02 -2.5778000e-05 -1.7660000e-05 /

C4H9-2+O(+m)=C4H8-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
69.79314815548514 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9439000e+00 7.0833000e-04 4.8878000e-04 /
CHEB / 2.0857000e+00 -6.7987000e-04 -4.6669000e-04 /
CHEB / 6.7271000e-01 -1.4570000e-04 -1.0307000e-04 /
CHEB / 2.2119000e-01 7.0853000e-05 4.7531000e-05 /
CHEB / 6.2420000e-02 5.2778000e-05 3.7695000e-05 /

C4H9-2+O(+m)=MEKenol+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
72.2231176688068 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3995000e+00 6.8135000e-04 4.6995000e-04 /
CHEB / 2.5453000e+00 -6.4984000e-04 -4.4572000e-04 /
CHEB / 7.9823000e-01 -1.4726000e-04 -1.0417000e-04 /
CHEB / 2.6780000e-01 6.8964000e-05 4.6243000e-05 /
CHEB / 8.2280000e-02 5.2358000e-05 3.7387000e-05 /

C4H9-2+O(+m)=sC4H8O+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
64.79376975400058 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4145000e+00 -2.1874000e-03 -1.5715000e-03 /
CHEB / 2.8067000e+00 1.9486000e-03 1.4013000e-03 /
CHEB / 9.2682000e-01 7.8048000e-04 5.6475000e-04 /
CHEB / 3.3105000e-01 -3.2014000e-04 -2.3639000e-04 /
CHEB / 1.0995000e-01 -2.8395000e-04 -2.0642000e-04 /

C4H9-2+O(+m)=CH3+C3H6O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
86.06156849650532 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1833000e+01 -1.6899000e-06 -1.1763000e-06 /
CHEB / 1.5492000e-01 1.6469000e-07 1.1464000e-07 /
CHEB / 8.8955000e-02 9.9176000e-07 6.9035000e-07 /
CHEB / 1.9926000e-02 5.6172000e-07 3.9101000e-07 /
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CHEB / -6.3639000e-03 1.5349000e-07 1.0684000e-07 /

C4H9-2+O(+m)=CH3CHO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
87.45093744148961 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3166000e+01 1.3717000e-07 9.5481000e-08 /
CHEB / -2.2282000e-01 1.9558000e-07 1.3614000e-07 /
CHEB / -4.2219000e-02 1.1592000e-07 8.0688000e-08 /
CHEB / -2.9910000e-02 6.7217000e-08 4.6788000e-08 /
CHEB / -2.4562000e-02 4.3639000e-08 3.0376000e-08 /

C4H9-2+O(+m)=MEK+H(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -82.42206370735542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2865000e+00 -2.5146000e-06 -1.7501000e-06 /
CHEB / 9.5539000e-01 2.7497000e-07 1.9115000e-07 /
CHEB / 3.2407000e-01 1.4733000e-06 1.0254000e-06 /
CHEB / 1.0986000e-01 8.1690000e-07 5.6872000e-07 /
CHEB / 3.2243000e-02 2.1133000e-07 1.4714000e-07 /

C4H9-2+O(+m)=H2CCCH3[OH]+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
81.83214586997454 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5145000e+00 -2.5076000e-05 -1.8904000e-05 /
CHEB / 2.3848000e+00 -3.1576000e-05 -2.0680000e-05 /
CHEB / 9.0247000e-01 3.6338000e-05 2.5534000e-05 /
CHEB / 3.7796000e-01 3.0887000e-05 2.1784000e-05 /
CHEB / 1.5307000e-01 1.6043000e-06 8.2387000e-07 /

C4H9-2+O(+m)=C2H5O-2+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
77.0120747844305 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3349000e+00 -5.3523000e-04 -4.0603000e-04 /
CHEB / 1.4482000e+00 3.9599000e-04 2.9622000e-04 /
CHEB / 5.2935000e-01 3.7815000e-04 2.9240000e-04 /
CHEB / 2.1310000e-01 -1.0401000e-04 -8.0392000e-05 /
CHEB / 8.5475000e-02 -1.6915000e-04 -1.3063000e-04 /

C4H9-2+O(+m)=C4H7-14+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CH[OH]C2H5)      deltaHrxn(T=298K) = -
87.2113228610684 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9279000e+00 -1.4048000e-02 -9.7872000e-03 /
CHEB / 4.2497000e+00 1.2273000e-02 8.5540000e-03 /
CHEB / 1.4579000e+00 4.8217000e-03 3.3543000e-03 /
CHEB / 5.1965000e-01 -1.6598000e-03 -1.1568000e-03 /
CHEB / 1.7808000e-01 -1.5393000e-03 -1.0704000e-03 /

!PDepNetwork C4H9Oi1 + C4H9Oi2 + C4H9Oi3 + C4H9Oi4
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!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9Oi1           -18.28      86.11 28.03 33.68 38.81 43.16 49.99
      55.12 63.33  !MRH
!     C4H9Oi3           -24.24      84.93 27.12 33.12 38.42 42.88 49.87
      55.11 63.43  !MRH
!     C4H9Oi2           -22.94      84.64 27.11 32.27 37.18 41.54 48.7
      54.18 62.91  !MRH
!     C4H9Oi4           -15.78      80.19 26.32 32.81 38.45 43.15 50.5
      55.97 64.52  !MRH
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H8O-i1          -38.26      82.01 24.81 30.17 35.04 39.27 46.13
      51.21 58.97 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H6O-enol        -34.7 70.85 20.67 24.56 28.02 30.98 35.68 39.25
      45.02
!     C4H8O-i2          -45.93      79.05 25.53 31.25 36.25 40.42 46.96
      51.79 59.42 null
!     C4H8O-i3          -51.2 79.65 23.57 29.46 34.96 39.45 46.7  51.93
      57.55 null
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     iC4H9       19.15 76.39 23.23 28.98 34.04 38.33 45.13 50.31 58.58
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C3H6+CH2OH=C4H9Oi1      2.4827386e+10      0.24400
1.0487500e+04
!     C3H6O-enol2+CH3=C4H9Oi1       1.3600000e+12      0.00000
1.0100000e+04
!     C4H8O-i1+H=C4H9Oi1            1.1700000e+13      0.00000
4.7000000e+03
!     C4H9Oi1=C4H9Oi3               2.1620731e+09      0.93000
3.2050000e+04
!     CH3+C3H6O-enol=C4H9Oi3        1.3600000e+12      0.00000
1.0100000e+04
!     C4H8O-i2+H=C4H9Oi3            1.0000000e+13      0.00000
2.9000000e+03
!     C4H8O-i3+H=C4H9Oi3            2.3501400e+11      0.30815
4.9629937e+03
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!     C4H9Oi2=C4H9Oi3               5.8800000e+08      1.27000
3.0100000e+04
!     C4H8O-i1+H=C4H9Oi2            4.9400000e+13      0.00000
1.5000000e+03
!     iC4H8+OH=C4H9Oi2         2.7100000e+12      0.00000
0.0000000e+00
!     C4H8O-i2+H=C4H9Oi2            1.0000000e+13      0.00000
2.9000000e+03
!     C4H9Oi4=C4H9Oi2               7.8893489e+08      1.25667
3.9395000e+04
!     C3H7-2+CH2O=C4H9Oi4      1.0000000e+11      0.00000
1.1900000e+04
!     C4H8O-i3+H=C4H9Oi4            1.0000000e+11      0.00000
1.1900000e+04
!     C4H9Oi4=C4H9Oi1               3.6000000e+12      0.00000
2.9400000e+04
!     C4H9Oi4=C4H9Oi3               8.1282219e+08      1.13906
3.4790987e+04
!     iC4H9+O=C4H9Oi4          1.0000000e+13      0.00000
0.0000000e+00
!     C4H9Oi1=C4H9Oi2               6.2339791e+09      0.93630
3.7689907e+04

C4H9Oi1(+m)=C4H9Oi3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -5.9592491593059265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5169000e+00 7.3296000e-01 -7.2053000e-02 /
CHEB / 5.1254000e+00 1.0365000e+00 -4.9374000e-02 /
CHEB / -4.3111000e+00 2.5959000e-01 5.4683000e-02 /
CHEB / -2.5866000e+00 -2.4195000e-01 4.8949000e-02 /
CHEB / -1.1891000e+00 -3.2693000e-01 -1.1365000e-02 /

C4H9Oi1(+m)=C4H9Oi2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_2H     Cs_H_out       deltaHrxn(T=298K) = -
4.6594343041085615 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8576000e+00 1.0087000e+00 -6.9520000e-02 /
CHEB / 6.8098000e+00 1.0548000e+00 1.5696000e-02 /
CHEB / -4.2583000e+00 2.2487000e-02 9.7994000e-02 /
CHEB / -2.5153000e+00 -3.0939000e-01 -1.9453000e-03 /
CHEB / -1.1514000e+00 -3.1578000e-01 -3.8312000e-02 /

C4H9Oi2(+m)=C4H9Oi3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    Others-C_rad_out_Cs2    Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -1.299814855197365 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4428000e+00 6.4201000e-01 -5.4152000e-02 /
CHEB / 4.5601000e+00 9.1245000e-01 -3.5937000e-02 /
CHEB / -4.3882000e+00 1.9726000e-01 5.4843000e-02 /
CHEB / -2.6357000e+00 -2.8313000e-01 5.1678000e-02 /
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CHEB / -1.1835000e+00 -3.5023000e-01 -8.8328000e-03 /

C4H9Oi4(+m)=C4H9Oi1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration exact:  R4H_SSS
O_rad_out     Cs_H_out_2H           deltaHrxn(T=298K) = -
2.5000345150457832 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2510000e+00 9.2632000e-01 -9.7260000e-02 /
CHEB / 3.7856000e+00 9.2135000e-01 3.5437000e-02 /
CHEB / -4.1846000e+00 2.1020000e-02 6.6423000e-02 /
CHEB / -2.3348000e+00 -3.3519000e-01 4.7475000e-03 /
CHEB / -1.0255000e+00 -2.9498000e-01 -3.4488000e-02 /

C4H9Oi4(+m)=C4H9Oi3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    O_rad_out     Cs_H_out_H/(NonDeC/Cs/Cs)
      deltaHrxn(T=298K) = -8.45928367435171 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7445000e+00 1.4621000e+00 -1.2921000e-01 /
CHEB / 5.3025000e+00 9.4032000e-01 6.1490000e-02 /
CHEB / -4.5390000e+00 2.9889000e-03 6.6039000e-02 /
CHEB / -2.5843000e+00 -3.0201000e-01 -1.2407000e-02 /
CHEB / -1.1206000e+00 -2.9332000e-01 -3.0171000e-02 /

C4H9Oi4(+m)=C4H9Oi2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R3H_SS    O_rad_out     Cs_H_out         deltaHrxn(T=298K) = -
7.159468819154345 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9949000e+00 1.8430000e+00 -3.1091000e-03 /
CHEB / 6.8480000e+00 8.1448000e-01 1.2120000e-02 /
CHEB / -4.3895000e+00 -2.1356000e-01 6.0114000e-02 /
CHEB / -2.5010000e+00 -3.3464000e-01 -3.4472000e-02 /
CHEB / -1.0870000e+00 -2.7807000e-01 -3.9843000e-02 /

C3H6+CH2OH(+m)=C4H9Oi1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/H2     C_rad/H2/O         deltaHrxn(T=298K) = -
20.67811158639114 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7029000e+00 6.6498000e-01 -4.5149000e-02 /
CHEB / -2.2228000e-01 1.0077000e+00 -2.3128000e-02 /
CHEB / -2.7479000e+00 4.0631000e-01 5.2457000e-02 /
CHEB / -1.6520000e+00 -1.3856000e-02 4.8253000e-02 /
CHEB / -8.1163000e-01 -1.3953000e-01 4.4161000e-03 /

C3H6+CH2OH(+m)=C4H9Oi3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -26.637360745697066
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5988000e-01 -3.3851000e-01 -1.6427000e-01 /
CHEB / 2.1038000e+00 2.1805000e+00 -3.5096000e-02 /
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CHEB / -2.9996000e+00 6.4734000e-01 1.3142000e-01 /
CHEB / -1.9969000e+00 -9.5249000e-02 6.4989000e-02 /
CHEB / -9.4472000e-01 -2.1490000e-01 -1.4847000e-02 /

C3H6+CH2OH(+m)=C4H9Oi2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -25.3375458904997
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3785000e+00 1.7675000e-01 -2.5103000e-01 /
CHEB / 3.2133000e+00 1.9415000e+00 1.5101000e-01 /
CHEB / -2.8408000e+00 3.8139000e-01 1.1726000e-01 /
CHEB / -1.8611000e+00 -1.3088000e-01 -9.6093000e-03 /
CHEB / -8.9067000e-01 -1.7548000e-01 -3.5125000e-02 /

C3H6+CH2OH(+m)=C4H9Oi4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -18.178077071345356
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8366000e-01 1.0428000e-01 -1.9330000e-01 /
CHEB / 1.6458000e+00 1.8109000e+00 1.1849000e-01 /
CHEB / -2.7343000e+00 3.2710000e-01 9.7016000e-02 /
CHEB / -1.6798000e+00 -1.4916000e-01 1.6511000e-02 /
CHEB / -7.6495000e-01 -1.7410000e-01 -1.7938000e-02 /

C3H6+CH2OH(+m)=CH3+C3H6O-enol(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -1.8503179914947339
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6899000e+00 -1.9631000e+00 -2.0989000e-01 /
CHEB / 7.6456000e+00 2.0830000e+00 8.8100000e-02 /
CHEB / -5.3514000e-02 2.4111000e-01 1.7547000e-01 /
CHEB / -2.2693000e-01 -2.3886000e-01 1.7791000e-02 /
CHEB / -4.6587000e-02 -1.4829000e-01 -4.4915000e-02 /

C3H6+CH2OH(+m)=C3H7-2+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -2.6094950871149223
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7925000e+00 -1.4318000e+00 -2.1685000e-01 /
CHEB / 6.3131000e+00 1.5873000e+00 1.6959000e-01 /
CHEB / -1.1733000e-01 8.6987000e-02 8.9933000e-02 /
CHEB / -1.5330000e-01 -1.7427000e-01 -8.9834000e-04 /
CHEB / -1.9428000e-02 -9.6402000e-02 -2.8632000e-02 /

C3H6O-enol2+CH3(+m)=C4H9Oi1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/Nd_Cd/H2     C_methyl          deltaHrxn(T=298K) = -
24.59705949051043 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7005000e+00 8.4016000e-01 -8.5851000e-02 /
CHEB / -6.9490000e-01 1.1605000e+00 -2.4467000e-02 /
CHEB / -2.8676000e+00 4.0520000e-01 7.3054000e-02 /
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CHEB / -1.6542000e+00 -4.0891000e-02 5.1122000e-02 /
CHEB / -8.0107000e-01 -1.4883000e-01 -9.1320000e-04 /

C3H6O-enol2+CH3(+m)=C4H9Oi3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -30.556308649816355
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8635000e+00 -1.2545000e-01 -2.1441000e-01 /
CHEB / 1.1982000e+00 2.2928000e+00 -1.9507000e-02 /
CHEB / -3.0676000e+00 6.2843000e-01 1.4417000e-01 /
CHEB / -1.9763000e+00 -1.0860000e-01 6.0831000e-02 /
CHEB / -9.3047000e-01 -2.1388000e-01 -1.7137000e-02 /

C3H6O-enol2+CH3(+m)=C4H9Oi2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -29.25649379461899
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1861000e-01 4.3186000e-01 -3.1191000e-01 /
CHEB / 2.1741000e+00 1.9990000e+00 1.8658000e-01 /
CHEB / -2.8620000e+00 3.6713000e-01 1.1653000e-01 /
CHEB / -1.8437000e+00 -1.3869000e-01 -1.3626000e-02 /
CHEB / -8.7700000e-01 -1.7324000e-01 -3.5141000e-02 /

C3H6O-enol2+CH3(+m)=C4H9Oi4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -22.097024975464645
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8451000e-01 4.4256000e-01 -2.5187000e-01 /
CHEB / 8.4511000e-01 1.7729000e+00 1.5538000e-01 /
CHEB / -2.7869000e+00 3.2771000e-01 9.2369000e-02 /
CHEB / -1.6565000e+00 -1.5262000e-01 1.8439000e-02 /
CHEB / -7.5092000e-01 -1.7538000e-01 -1.7375000e-02 /

C3H6O-enol2+CH3(+m)=C3H6+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -3.9189479041192903
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7285000e+00 -1.0023000e+00 -1.1098000e-01 /
CHEB / 4.3956000e+00 1.0631000e+00 4.1648000e-02 /
CHEB / -2.0505000e-01 1.3783000e-01 1.0087000e-01 /
CHEB / -1.7357000e-01 -1.3704000e-01 1.1774000e-02 /
CHEB / -4.6212000e-02 -8.6698000e-02 -3.1687000e-02 /

C3H6O-enol2+CH3(+m)=CH3+C3H6O-enol(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9Oi1) deltaHrxn(T=298K) = -5.769265895614023
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4020000e+00 -1.8536000e+00 -2.3543000e-01 /
CHEB / 6.7939000e+00 2.0134000e+00 1.2557000e-01 /
CHEB / 8.1282000e-03 1.7429000e-01 1.7379000e-01 /
CHEB / -1.6289000e-01 -2.3923000e-01 3.8660000e-03 /
CHEB / -2.4884000e-02 -1.2900000e-01 -4.8916000e-02 /
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C3H6O-enol2+CH3(+m)=C4H8O-i3+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -5.419144547457087
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3327000e+00 -1.9492000e+00 -2.1298000e-01 /
CHEB / 6.7222000e+00 2.0486000e+00 8.9047000e-02 /
CHEB / 5.1641000e-03 2.6017000e-01 1.7481000e-01 /
CHEB / -1.7712000e-01 -2.2794000e-01 2.2708000e-02 /
CHEB / -2.7561000e-02 -1.5291000e-01 -4.3731000e-02 /

C3H6O-enol2+CH3(+m)=C3H7-2+CH2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -6.528442991234211
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4311000e+00 -1.2864000e+00 -2.3001000e-01 /
CHEB / 5.5432000e+00 1.4529000e+00 1.9299000e-01 /
CHEB / -5.1905000e-02 5.0109000e-02 8.4997000e-02 /
CHEB / -9.5712000e-02 -1.6853000e-01 -8.8999000e-03 /
CHEB / -2.6639000e-03 -7.9583000e-02 -3.1844000e-02 /

C4H8O-i1+H(+m)=C4H9Oi1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond exact:
Cd/Nd2_Cd/H2     H_rad        deltaHrxn(T=298K) = -32.11647598727519
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7944000e+00 9.1705000e-01 -1.0613000e-01 /
CHEB / -2.6125000e+00 1.2080000e+00 -1.8849000e-02 /
CHEB / -2.8742000e+00 4.0135000e-01 8.1368000e-02 /
CHEB / -1.6646000e+00 -4.9173000e-02 5.1469000e-02 /
CHEB / -7.9679000e-01 -1.5114000e-01 -2.7277000e-03 /

C4H8O-i1+H(+m)=C4H9Oi3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -38.075725146581114
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8861000e+00 -1.2001000e-01 -2.1783000e-01 /
CHEB / -2.0752000e+00 2.2927000e+00 -8.9942000e-03 /
CHEB / -3.1650000e+00 6.4141000e-01 1.4677000e-01 /
CHEB / -2.0555000e+00 -1.1788000e-01 6.0660000e-02 /
CHEB / -9.6315000e-01 -2.2863000e-01 -2.0945000e-02 /

C4H8O-i1+H(+m)=C4H9Oi2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/Nd2     H_rad        deltaHrxn(T=298K) = -36.77591029138375
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0236000e+01 1.1687000e+00 -1.7081000e-01 /
CHEB / -4.4175000e+00 1.4377000e+00 -3.0740000e-02 /
CHEB / -3.3092000e+00 4.0455000e-01 1.0852000e-01 /
CHEB / -1.8572000e+00 -1.2321000e-01 6.4719000e-02 /
CHEB / -8.4496000e-01 -2.0493000e-01 -5.8997000e-03 /
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C4H8O-i1+H(+m)=C4H9Oi4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -29.616441472229404
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4583000e+00 5.9710000e-01 -2.6882000e-01 /
CHEB / -1.1256000e+00 1.7783000e+00 1.7820000e-01 /
CHEB / -2.7605000e+00 3.5371000e-01 9.9782000e-02 /
CHEB / -1.6454000e+00 -1.3722000e-01 2.3434000e-02 /
CHEB / -7.3659000e-01 -1.6569000e-01 -1.5233000e-02 /

C4H8O-i1+H(+m)=C3H6+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -11.43836440088405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0015000e+01 -9.7082000e-01 -1.2018000e-01 /
CHEB / 2.4501000e+00 1.0413000e+00 5.4706000e-02 /
CHEB / -1.5369000e-01 1.1968000e-01 1.0048000e-01 /
CHEB / -1.5829000e-01 -1.3560000e-01 6.9140000e-03 /
CHEB / -3.5528000e-02 -8.0573000e-02 -3.2673000e-02 /

C4H8O-i1+H(+m)=C3H6O-enol2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -7.519416496764755
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6627000e+00 -9.1152000e-01 -1.3310000e-01 /
CHEB / 3.2148000e+00 1.0035000e+00 7.6122000e-02 /
CHEB / -2.1871000e-02 8.0041000e-02 9.8057000e-02 /
CHEB / -1.1440000e-01 -1.3255000e-01 -3.3109000e-03 /
CHEB / -2.2090000e-02 -6.6854000e-02 -3.3761000e-02 /

C4H8O-i1+H(+m)=CH3+C3H6O-enol(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -13.288682392378782
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1152000e+00 -1.8426000e+00 -2.4590000e-01 /
CHEB / 3.8759000e+00 2.0069000e+00 1.3552000e-01 /
CHEB / -9.7080000e-02 1.7632000e-01 1.7894000e-01 /
CHEB / -2.6451000e-01 -2.4959000e-01 1.8272000e-03 /
CHEB / -7.1343000e-02 -1.3360000e-01 -5.4170000e-02 /

C4H8O-i1+H(+m)=C4H8O-i2+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -7.669293951907498
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0719000e+01 -9.3862000e-01 -1.3547000e-01 /
CHEB / 2.2903000e+00 1.0271000e+00 7.0044000e-02 /
CHEB / 4.3125000e-02 9.6011000e-02 1.0926000e-01 /
CHEB / -1.3485000e-01 -1.4113000e-01 -5.1835000e-05 /
CHEB / -4.9774000e-02 -7.5331000e-02 -3.9814000e-02 /
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C4H8O-i1+H(+m)=C4H8O-i3+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -12.93856104422185
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1056000e+00 -1.9568000e+00 -2.2569000e-01 /
CHEB / 3.7213000e+00 2.0661000e+00 1.0081000e-01 /
CHEB / -8.6820000e-02 2.6239000e-01 1.8108000e-01 /
CHEB / -2.7599000e-01 -2.4419000e-01 2.0214000e-02 /
CHEB / -7.1802000e-02 -1.6006000e-01 -4.8750000e-02 /

C4H8O-i1+H(+m)=iC4H8+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -7.3689848683775026
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2105000e+01 -9.5296000e-01 -1.3271000e-01 /
CHEB / 1.2694000e+00 1.0370000e+00 6.4839000e-02 /
CHEB / -2.1491000e-01 1.0711000e-01 1.1034000e-01 /
CHEB / -2.2139000e-01 -1.4414000e-01 3.0925000e-03 /
CHEB / -8.2841000e-02 -8.0609000e-02 -4.0269000e-02 /

C4H8O-i1+H(+m)=C3H7-2+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -14.04785948799897
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8803000e+00 -1.2278000e+00 -2.3422000e-01 /
CHEB / 3.8234000e+00 1.3980000e+00 2.0302000e-01 /
CHEB / 2.0188000e-01 3.7971000e-02 8.1735000e-02 /
CHEB / 4.1671000e-02 -1.6808000e-01 -1.3632000e-02 /
CHEB / 6.6499000e-02 -7.4861000e-02 -3.3203000e-02 /

CH3+C3H6O-enol(+m)=C4H9Oi1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -18.827793594896406
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0328000e-01 -3.4768000e-01 -1.4471000e-01 /
CHEB / 3.2442000e+00 2.1900000e+00 -1.7789000e-02 /
CHEB / -2.5963000e+00 6.5188000e-01 1.4004000e-01 /
CHEB / -1.7727000e+00 -9.1702000e-02 6.6851000e-02 /
CHEB / -8.7214000e-01 -2.0888000e-01 -1.6170000e-02 /

CH3+C3H6O-enol(+m)=C4H9Oi3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) C_methyl     Cd/H/Nd_Cd/H/Nd         deltaHrxn(T=298K) = -
24.787042754202332 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5925000e+00 7.6233000e-01 -5.8735000e-02 /
CHEB / -1.1892000e+00 1.2082000e+00 -5.5122000e-02 /
CHEB / -3.3420000e+00 5.5446000e-01 3.8910000e-02 /
CHEB / -1.9888000e+00 3.8950000e-02 5.8931000e-02 /
CHEB / -9.4651000e-01 -1.4940000e-01 1.6820000e-02 /
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CH3+C3H6O-enol(+m)=C4H9Oi2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -23.487227899004967
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0742000e+00 -2.5476000e-01 -1.7559000e-01 /
CHEB / 1.6350000e+00 2.2626000e+00 -2.2639000e-02 /
CHEB / -3.0591000e+00 6.6917000e-01 1.4450000e-01 /
CHEB / -2.0182000e+00 -1.0050000e-01 6.7145000e-02 /
CHEB / -9.6248000e-01 -2.2519000e-01 -1.8261000e-02 /

CH3+C3H6O-enol(+m)=C4H9Oi4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -16.327759079850622
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6626000e+00 5.6988000e-01 -1.7635000e-01 /
CHEB / 3.8505000e+00 1.7645000e+00 1.3973000e-01 /
CHEB / -2.6272000e+00 3.9836000e-01 6.8797000e-02 /
CHEB / -1.6532000e+00 -9.1527000e-02 1.7726000e-02 /
CHEB / -7.7370000e-01 -1.6426000e-01 -5.4054000e-03 /

CH3+C3H6O-enol(+m)=C3H7-2+CH2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -0.7591770956201884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8293000e-02 -1.3207000e+00 -1.9929000e-01 /
CHEB / 8.6897000e+00 1.4561000e+00 1.4783000e-01 /
CHEB / 2.0483000e-01 9.8690000e-02 8.8805000e-02 /
CHEB / -2.7746000e-02 -1.7039000e-01 8.2325000e-03 /
CHEB / 1.3551000e-02 -9.4527000e-02 -3.1146000e-02 /

C4H8O-i2+H(+m)=C4H9Oi1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -24.44718203536769
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1651000e+00 -4.3777000e-01 -1.2037000e-01 /
CHEB / 1.5519000e+00 2.1058000e+00 -1.1431000e-02 /
CHEB / -2.5197000e+00 6.2518000e-01 1.3188000e-01 /
CHEB / -1.7454000e+00 -1.1073000e-01 6.3527000e-02 /
CHEB / -8.5076000e-01 -2.2037000e-01 -1.6619000e-02 /

C4H8O-i2+H(+m)=C4H9Oi3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/Nd2_Cd/H/Nd     H_rad       deltaHrxn(T=298K) = -
30.406431194673615 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4554000e+00 6.5386000e-01 -4.3299000e-02 /
CHEB / -3.2597000e+00 1.0501000e+00 -4.1263000e-02 /
CHEB / -3.1770000e+00 4.9381000e-01 3.4032000e-02 /
CHEB / -1.9238000e+00 2.8740000e-02 5.5175000e-02 /
CHEB / -9.1529000e-01 -1.5381000e-01 1.9645000e-02 /
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C4H8O-i2+H(+m)=C4H9Oi2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H/Nd_Cd/Nd2     H_rad       deltaHrxn(T=298K) = -
29.10661633947625 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4151000e+00 7.5818000e-01 -6.2477000e-02 /
CHEB / -3.3588000e+00 1.1323000e+00 -3.8970000e-02 /
CHEB / -3.0961000e+00 4.2272000e-01 5.9396000e-02 /
CHEB / -1.8014000e+00 -5.8118000e-02 5.7225000e-02 /
CHEB / -8.3848000e-01 -1.7868000e-01 4.4096000e-03 /

C4H8O-i2+H(+m)=C4H9Oi4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -21.947147520321906
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2999000e-01 4.5490000e-01 -1.5739000e-01 /
CHEB / 2.2049000e+00 1.7196000e+00 1.4611000e-01 /
CHEB / -2.5737000e+00 3.6519000e-01 6.8554000e-02 /
CHEB / -1.6240000e+00 -1.1196000e-01 1.0619000e-02 /
CHEB / -7.5012000e-01 -1.7257000e-01 -7.0295000e-03 /

C4H8O-i2+H(+m)=C3H6+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -3.7690704489765507
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1797000e+00 -1.9902000e+00 -1.9506000e-01 /
CHEB / 6.3450000e+00 2.1072000e+00 7.7527000e-02 /
CHEB / -1.1823000e-01 2.5312000e-01 1.6753000e-01 /
CHEB / -2.4425000e-01 -2.4561000e-01 1.7937000e-02 /
CHEB / -4.8083000e-02 -1.5303000e-01 -4.2297000e-02 /

C4H8O-i2+H(+m)=C3H6O-enol2+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = 0.14987745514273598
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8361000e+00 -1.8746000e+00 -2.2246000e-01 /
CHEB / 7.0809000e+00 2.0371000e+00 1.1604000e-01 /
CHEB / 7.1778000e-03 1.8015000e-01 1.6744000e-01 /
CHEB / -1.8043000e-01 -2.4781000e-01 4.0503000e-03 /
CHEB / -3.0430000e-02 -1.3281000e-01 -4.6905000e-02 /

C4H8O-i2+H(+m)=CH3+C3H6O-enol(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -5.619388440471283
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6589000e+00 -1.1536000e+00 -7.2878000e-02 /
CHEB / 3.5422000e+00 1.1353000e+00 -1.3505000e-02 /
CHEB / -2.2062000e-01 2.6677000e-01 9.3780000e-02 /
CHEB / -2.2897000e-01 -1.3627000e-01 4.4607000e-02 /
CHEB / -5.3361000e-02 -1.3117000e-01 -2.2540000e-02 /
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C4H8O-i2+H(+m)=C4H8O-i3+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -5.269267092314351
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8969000e+00 -1.2141000e+00 -5.9396000e-02 /
CHEB / 3.0873000e+00 1.1292000e+00 -2.5423000e-02 /
CHEB / -1.6529000e-01 3.4200000e-01 7.7903000e-02 /
CHEB / -2.4262000e-01 -1.0544000e-01 5.5589000e-02 /
CHEB / -5.5464000e-02 -1.5001000e-01 -9.4379000e-03 /

C4H8O-i2+H(+m)=iC4H8+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = 0.3003090835299975
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0282000e+01 -1.0931000e+00 -8.9678000e-02 /
CHEB / 2.4887000e+00 1.1203000e+00 5.7729000e-03 /
CHEB / -2.7514000e-01 2.0477000e-01 1.0506000e-01 /
CHEB / -2.7162000e-01 -1.4680000e-01 3.0657000e-02 /
CHEB / -9.0029000e-02 -1.1345000e-01 -3.1977000e-02 /

C4H8O-i2+H(+m)=C3H7-2+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -6.378565536091472
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3273000e+00 -1.3468000e+00 -1.9242000e-01 /
CHEB / 6.9800000e+00 1.4916000e+00 1.4617000e-01 /
CHEB / 2.0143000e-01 9.7494000e-02 8.2130000e-02 /
CHEB / -3.9665000e-02 -1.8086000e-01 6.5951000e-03 /
CHEB / 8.5813000e-03 -9.7316000e-02 -2.9110000e-02 /

C4H8O-i3+H(+m)=C4H9Oi1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -19.177914943053338
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2831000e+00 -5.6313000e-01 -1.0747000e-01 /
CHEB / 3.0027000e+00 1.9874000e+00 -2.2542000e-02 /
CHEB / -2.5275000e+00 6.5507000e-01 1.1871000e-01 /
CHEB / -1.7567000e+00 -6.5290000e-02 7.0391000e-02 /
CHEB / -8.6282000e-01 -2.0678000e-01 -1.0229000e-02 /

C4H8O-i3+H(+m)=C4H9Oi3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) OCO     H_rad      deltaHrxn(T=298K) = -25.137164102359264
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1249000e+00 5.7384000e-01 -2.9512000e-02 /
CHEB / -2.4029000e+00 9.4222000e-01 -2.8507000e-02 /
CHEB / -3.0668000e+00 4.7927000e-01 2.6503000e-02 /
CHEB / -1.9103000e+00 6.2250000e-02 4.6573000e-02 /
CHEB / -9.2188000e-01 -1.2514000e-01 2.0172000e-02 /
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C4H8O-i3+H(+m)=C4H9Oi2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -23.8373492471619
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0038000e+00 -5.3707000e-01 -1.1790000e-01 /
CHEB / 1.1547000e+00 2.0500000e+00 -3.2471000e-02 /
CHEB / -2.9035000e+00 6.7344000e-01 1.2564000e-01 /
CHEB / -1.9965000e+00 -8.5069000e-02 7.4895000e-02 /
CHEB / -9.4759000e-01 -2.2953000e-01 -1.1938000e-02 /

C4H8O-i3+H(+m)=C4H9Oi4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) CO/H/Nd_O     H_rad      deltaHrxn(T=298K) = -
16.677880428007555 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5388000e+00 8.7747000e-01 -6.6426000e-02 /
CHEB / -5.6483000e-01 1.0508000e+00 2.5160000e-02 /
CHEB / -2.9498000e+00 2.4319000e-01 6.3305000e-02 /
CHEB / -1.5660000e+00 -1.1270000e-01 1.2951000e-02 /
CHEB / -6.6443000e-01 -1.3175000e-01 -1.8447000e-02 /

C4H8O-i3+H(+m)=C3H6+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = 1.5001966433378002
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0550000e+00 -2.0693000e+00 -1.8389000e-01 /
CHEB / 7.6957000e+00 2.1116000e+00 5.1414000e-02 /
CHEB / -2.2445000e-01 3.3989000e-01 1.7022000e-01 /
CHEB / -2.9855000e-01 -2.1652000e-01 3.6673000e-02 /
CHEB / -5.7529000e-02 -1.7103000e-01 -3.7319000e-02 /

C4H8O-i3+H(+m)=CH3+C3H6O-enol(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -0.3501213481569323
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7152000e+00 -1.1842000e+00 -6.5959000e-02 /
CHEB / 4.8619000e+00 1.1342000e+00 -1.9975000e-02 /
CHEB / -2.6235000e-01 3.0517000e-01 8.6077000e-02 /
CHEB / -2.4996000e-01 -1.2315000e-01 5.0701000e-02 /
CHEB / -4.8348000e-02 -1.4273000e-01 -1.6077000e-02 /

C4H8O-i3+H(+m)=C3H7-2+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -1.1092984437771207
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5394000e+00 -7.0653000e-01 -1.2904000e-01 /
CHEB / 4.8999000e+00 8.5121000e-01 1.1458000e-01 /
CHEB / -1.1209000e-01 -2.8789000e-02 5.3756000e-02 /
CHEB / -4.4032000e-02 -1.1454000e-01 -2.3234000e-02 /
CHEB / 2.6460000e-02 -3.1910000e-02 -2.2790000e-02 /
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iC4H8+OH(+m)=C4H9Oi1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -24.747491118897685
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2120000e+00 -1.6268000e-01 -1.8303000e-01 /
CHEB / 2.0270000e+00 1.8513000e+00 1.1071000e-01 /
CHEB / -2.5493000e+00 3.9561000e-01 1.3487000e-01 /
CHEB / -1.6866000e+00 -1.3054000e-01 1.0103000e-02 /
CHEB / -8.3588000e-01 -1.8384000e-01 -3.3282000e-02 /

iC4H8+OH(+m)=C4H9Oi3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -30.70674027820361
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8705000e+00 -5.5907000e-01 -1.1890000e-01 /
CHEB / -1.1082000e+00 2.0120000e+00 -3.4309000e-02 /
CHEB / -3.0090000e+00 6.5022000e-01 1.2255000e-01 /
CHEB / -2.0463000e+00 -9.8582000e-02 7.2793000e-02 /
CHEB / -9.7172000e-01 -2.3503000e-01 -1.2655000e-02 /

iC4H8+OH(+m)=C4H9Oi2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H2_Cd/Nd2     O_pri_rad           deltaHrxn(T=298K) = -
29.40692542300625 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0190000e+01 6.8580000e-01 -4.7418000e-02 /
CHEB / -4.3007000e+00 1.0495000e+00 -3.2039000e-02 /
CHEB / -3.0643000e+00 4.1321000e-01 5.1093000e-02 /
CHEB / -1.8050000e+00 -4.7785000e-02 5.4574000e-02 /
CHEB / -8.4959000e-01 -1.7554000e-01 7.3408000e-03 /

iC4H8+OH(+m)=C4H9Oi4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -22.2474566038519
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1839000e+00 7.4808000e-01 -6.8146000e-02 /
CHEB / 2.7772000e+00 1.4243000e+00 8.7249000e-02 /
CHEB / -2.5768000e+00 1.6109000e-01 7.4748000e-02 /
CHEB / -1.5862000e+00 -1.1681000e-01 -1.5713000e-02 /
CHEB / -7.3848000e-01 -1.4083000e-01 -2.0951000e-02 /

iC4H8+OH(+m)=C3H6+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -4.069379532506549
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4637000e+00 -1.6390000e+00 -2.8129000e-01 /
CHEB / 6.4655000e+00 1.8063000e+00 2.1159000e-01 /
CHEB / -1.2852000e-01 1.1706000e-01 1.4105000e-01 /
CHEB / -2.5342000e-01 -2.0915000e-01 -1.9678000e-02 /
CHEB / -8.5288000e-02 -1.0604000e-01 -4.3115000e-02 /
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iC4H8+OH(+m)=C3H6O-enol2+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -0.15043162838725976
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1667000e+00 -1.5304000e+00 -3.0177000e-01 /
CHEB / 7.1478000e+00 1.7273000e+00 2.4474000e-01 /
CHEB / 9.6855000e-03 6.1981000e-02 1.3505000e-01 /
CHEB / -2.0043000e-01 -2.0583000e-01 -3.0221000e-02 /
CHEB / -6.8575000e-02 -8.8856000e-02 -4.5002000e-02 /

iC4H8+OH(+m)=CH3+C3H6O-enol(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -5.919697524001279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2517000e+00 -2.0362000e+00 -2.0416000e-01 /
CHEB / 4.8918000e+00 2.1149000e+00 7.1763000e-02 /
CHEB / -2.9699000e-01 3.0952000e-01 1.8060000e-01 /
CHEB / -3.7654000e-01 -2.3978000e-01 2.9615000e-02 /
CHEB / -1.1265000e-01 -1.7267000e-01 -4.4890000e-02 /

iC4H8+OH(+m)=C4H8O-i3+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -5.569576175844347
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3985000e+00 -2.1795000e+00 -1.7159000e-01 /
CHEB / 4.6111000e+00 2.1650000e+00 2.9324000e-02 /
CHEB / -2.6630000e-01 4.2507000e-01 1.7228000e-01 /
CHEB / -4.1245000e-01 -2.1117000e-01 4.8127000e-02 /
CHEB / -1.2584000e-01 -1.9553000e-01 -3.5174000e-02 /

iC4H8+OH(+m)=C3H7-2+CH2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -6.678874619621471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5127000e+00 -9.8722000e-01 -2.1953000e-01 /
CHEB / 7.2567000e+00 1.1461000e+00 1.9673000e-01 /
CHEB / 1.3870000e-01 -1.2046000e-03 7.7821000e-02 /
CHEB / -7.0336000e-02 -1.3061000e-01 -2.8182000e-02 /
CHEB / -3.0698000e-02 -5.6217000e-02 -2.8202000e-02 /

C3H7-2+CH2O(+m)=C4H9Oi1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -18.068616499276217
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5870000e-01 2.3722000e-02 -1.7930000e-01 /
CHEB / 2.4435000e+00 1.8358000e+00 1.0763000e-01 /
CHEB / -2.5983000e+00 3.7821000e-01 9.9960000e-02 /
CHEB / -1.6539000e+00 -1.1293000e-01 2.2571000e-02 /
CHEB / -7.9865000e-01 -1.6406000e-01 -1.4497000e-02 /
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```
C3H7-2+CH2O(+m)=C4H9Oi3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -24.027865658582144
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5468000e+00 4.2137000e-01 -2.0899000e-01 /
CHEB / 3.5089000e+00 1.8808000e+00 9.5302000e-02 /
CHEB / -2.9360000e+00 4.8786000e-01 8.6144000e-02 /
CHEB / -1.8847000e+00 -7.4403000e-02 4.0485000e-02 /
CHEB / -8.9471000e-01 -1.7739000e-01 -1.0786000e-03 /

C3H7-2+CH2O(+m)=C4H9Oi2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -22.72805080338478
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.4647000e+00 9.6811000e-01 -1.9413000e-01 /
CHEB / 4.7215000e+00 1.5880000e+00 1.4708000e-01 /
CHEB / -2.7798000e+00 2.4568000e-01 8.7483000e-02 /
CHEB / -1.7619000e+00 -9.9951000e-02 -1.6717000e-02 /
CHEB / -8.4196000e-01 -1.4794000e-01 -2.3114000e-02 /

C3H7-2+CH2O(+m)=C4H9Oi4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) C_rad/H/NonDeC     CO/H2_O           deltaHrxn(T=298K) = -
15.568581984230434 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3294000e+00 9.2754000e-01 -7.8779000e-02 /
CHEB / -5.6551000e-01 1.0621000e+00 3.1231000e-02 /
CHEB / -3.0090000e+00 2.3382000e-01 6.5204000e-02 /
CHEB / -1.6187000e+00 -1.1760000e-01 1.1685000e-02 /
CHEB / -7.0942000e-01 -1.3288000e-01 -1.9076000e-02 /

iC4H9+O(+m)=C4H9Oi1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1)      deltaHrxn(T=298K) = -97.06022136012147 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4937000e+00 1.3469000e+01 1.3954000e-01 /
CHEB / -2.1192000e+00 -1.9195000e+00 2.1266000e-01 /
CHEB / -2.1255000e+00 -1.3491000e+00 3.6652000e-01 /
CHEB / -1.4685000e+00 -4.2472000e-01 1.0865000e-01 /
CHEB / -9.2732000e-01 9.4803000e-02 -4.2699000e-02 /

iC4H9+O(+m)=C4H9Oi3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1)      deltaHrxn(T=298K) = -103.0194705194274 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7513000e+00 1.3519000e+01 -4.6536000e-01 /
CHEB / -3.4807000e+00 -1.5277000e+00 7.1658000e-01 /
CHEB / -2.9745000e+00 -1.0591000e+00 4.2561000e-01 /
CHEB / -1.8716000e+00 -4.1403000e-01 1.1004000e-01 /
CHEB / -1.0352000e+00 8.7266000e-03 -5.2280000e-02 /

iC4H9+O(+m)=C4H9Oi2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1)      deltaHrxn(T=298K) = -101.71965566423003 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -1.0310000e+01 1.4417000e+01 -3.4807000e-01 /
CHEB / -2.9227000e+00 -2.4454000e+00 7.0396000e-01 /
CHEB / -2.5367000e+00 -1.1830000e+00 2.6989000e-01 /
CHEB / -1.7021000e+00 -3.0880000e-01 9.8479000e-02 /
CHEB / -9.8942000e-01 6.7449000e-02 -6.5710000e-03 /

iC4H9+O(+m)=C4H9Oi4(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9Oi1) High-P Limit: Oa_R_Recombination estimate: (Average:)
C_rad/H2/Cs     Oa      deltaHrxn(T=298K) = -94.56018684507569 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2518000e+01 1.1217000e+01 1.5486000e+00 /
CHEB / -1.6297000e+00 4.0418000e-01 -7.8333000e-01 /
CHEB / -1.6858000e+00 -9.4043000e-01 -6.3416000e-02 /
CHEB / -1.0364000e+00 -6.8833000e-01 1.0536000e-01 /
CHEB / -6.3122000e-01 -2.5402000e-01 1.3348000e-01 /

iC4H9+O(+m)=C3H6+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -76.38210977373033
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7498000e+00 4.1874000e-04 2.9426000e-04 /
CHEB / 1.0306000e+00 -3.5690000e-04 -2.5122000e-04 /
CHEB / 2.6591000e-01 -1.2601000e-04 -8.8368000e-05 /
CHEB / 9.5306000e-02 2.9563000e-05 2.1051000e-05 /
CHEB / 3.3156000e-02 3.2717000e-05 2.3063000e-05 /

iC4H9+O(+m)=C3H6O-enol2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -72.46316186961104
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9890000e+00 -3.7606000e-04 -2.6583000e-04 /
CHEB / 1.3059000e+00 3.8139000e-04 2.7008000e-04 /
CHEB / 3.6044000e-01 6.3543000e-05 4.4685000e-05 /
CHEB / 1.3009000e-01 -4.9232000e-05 -3.5323000e-05 /
CHEB / 4.5449000e-02 -2.7227000e-05 -1.9154000e-05 /

iC4H9+O(+m)=C4H8O-i1+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -64.94374537284628
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7148000e+00 -1.6568000e-03 -1.1847000e-03 /
CHEB / 2.2341000e+00 1.6006000e-03 1.1523000e-03 /
CHEB / 7.0279000e-01 3.8558000e-04 2.6798000e-04 /
CHEB / 2.5659000e-01 -2.2569000e-04 -1.6493000e-04 /
CHEB / 8.5612000e-02 -1.4132000e-04 -9.8637000e-05 /

iC4H9+O(+m)=CH3+C3H6O-enol(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -78.23242776522507
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1833000e+00 -7.7921000e-04 -6.3814000e-04 /
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CHEB / 1.8987000e+00 9.1950000e-04 7.6688000e-04 /
CHEB / 5.4695000e-01 -3.8862000e-05 -4.4910000e-05 /
CHEB / 1.9531000e-01 -1.3578000e-04 -1.1594000e-04 /
CHEB / 6.6505000e-02 1.1549000e-05 1.2693000e-05 /

iC4H9+O(+m)=C4H8O-i2+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -72.6130393247538
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9340000e+00 -9.6162000e-05 -1.4451000e-04 /
CHEB / 2.5621000e+00 2.9819000e-04 3.1858000e-04 /
CHEB / 6.9339000e-01 -2.4907000e-04 -2.0238000e-04 /
CHEB / 2.3491000e-01 -3.0114000e-05 -3.3581000e-05 /
CHEB / 7.8790000e-02 7.1006000e-05 5.6608000e-05 /

iC4H9+O(+m)=C4H8O-i3+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -77.88230641706815
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9838000e+00 8.9653000e-06 6.2580000e-06 /
CHEB / 9.4477000e-01 -3.0067000e-08 -7.4767000e-09 /
CHEB / 2.7698000e-01 -5.2316000e-06 -3.6662000e-06 /
CHEB / 1.1025000e-01 -3.0118000e-06 -2.1188000e-06 /
CHEB / 4.2727000e-02 -5.7080000e-07 -3.9483000e-07 /

iC4H9+O(+m)=iC4H8+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -72.31273024122379
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7428000e+00 -8.9773000e-05 -1.3663000e-04 /
CHEB / 1.8301000e+00 4.1776000e-04 4.0490000e-04 /
CHEB / 4.7210000e-01 -4.3399000e-04 -3.4598000e-04 /
CHEB / 1.4690000e-01 1.0021000e-05 3.6985000e-06 /
CHEB / 4.1761000e-02 9.7619000e-05 7.6487000e-05 /

iC4H9+O(+m)=C3H7-2+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9Oi1)      deltaHrxn(T=298K) = -78.99160486084526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3159000e+01 -6.3901000e-07 -4.4499000e-07 /
CHEB / -1.4991000e-01 8.0251000e-07 5.5870000e-07 /
CHEB / -1.9124000e-02 9.4782000e-07 6.6000000e-07 /
CHEB / -2.3066000e-04 8.3042000e-08 5.7803000e-08 /
CHEB / -4.9814000e-03 -3.8652000e-07 -2.6921000e-07 /

!PDepNetwork OC[CH3]3 + HOC[CH2][CH3]2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OC[CH3]3          -23.14      76.55 26.22 32.91 38.66 43.41 50.9
      56.36 64.83 null
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!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!     acetone           -51.21      70.9  17.53 21.65 25.52 28.9  34.34
      38.41 44.77
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     tC4H9             14.3  76.21 21.71 26.64 31.62 36.12 43.55 49.22
      58.13
!Here are the path reactions and their high-P limit kinetics:
!     acetone+CH3=OC[CH3]3          3.1600000e+10      0.00000
1.1510000e+04
!     OC[CH3]3=HOC[CH2][CH3]2       3.8151000e+10      1.45000
4.2270000e+04
!     OH+iC4H8=HOC[CH2][CH3]2 2.7100000e+12      0.00000
0.0000000e+00
!     H2CCCH3[OH]+CH3=HOC[CH2][CH3]2      1.1200000e+12      0.00000
1.1200000e+04
!     O+tC4H9=OC[CH3]3        1.0000000e+13      0.00000
0.0000000e+00

OC[CH3]3(+m)=HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     Cs_H_out_2H
      deltaHrxn(T=298K) = -1.6002856661875207 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7113000e+01 7.0435000e+00 5.8705000e-02 /
CHEB / 1.0821000e+01 -7.9696000e-01 6.3151000e-02 /
CHEB / -3.1411000e+00 -7.7626000e-01 8.6078000e-02 /
CHEB / -1.7819000e+00 -3.3771000e-01 -1.0202000e-02 /
CHEB / -8.3752000e-01 -4.1194000e-04 -6.2049000e-02 /

acetone+CH3(+m)=OC[CH3]3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3) High-P Limit: R_Addition_MultipleBond exact:
CO/Nd2_O     C_methyl         deltaHrxn(T=298K) = -7.17912587356561
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1644000e+00 1.5646000e+00 -1.6433000e-01 /
CHEB / -8.1754000e-01 4.5600000e-01 1.7911000e-01 /
CHEB / -2.7958000e+00 9.0361000e-02 2.3043000e-02 /
CHEB / -1.2809000e+00 -8.3170000e-02 -2.9149000e-02 /
CHEB / -4.8729000e-01 -5.7665000e-02 -1.8848000e-02 /

acetone+CH3(+m)=HOC[CH2][CH3]2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -8.77941153975313
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7564000e+00 1.6329000e+00 -3.8152000e-01 /
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CHEB / 9.0295000e+00 9.3436000e-01 1.7640000e-01 /
CHEB / -2.3566000e+00 2.3698000e-01 8.5915000e-02 /
CHEB / -1.3792000e+00 -1.3077000e-01 2.0811000e-02 /
CHEB / -6.4785000e-01 -1.5860000e-01 -1.5688000e-02 /

OH+iC4H8(+m)=OC[CH3]3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -29.6066979206664
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9012000e+00 5.3801000e+00 2.7484000e-01 /
CHEB / 3.1679000e+00 9.4370000e-02 1.1120000e-01 /
CHEB / -1.6754000e+00 -4.0380000e-01 1.3311000e-01 /
CHEB / -1.1183000e+00 -2.2654000e-01 1.2958000e-02 /
CHEB / -6.4468000e-01 1.0756000e-02 -4.8946000e-02 /

OH+iC4H8(+m)=HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) O_pri_rad     Cd/Nd2_Cd/H2       deltaHrxn(T=298K)
= -31.206983586853923 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9837000e+00 7.7577000e-01 -5.5027000e-02 /
CHEB / -4.3151000e+00 1.0890000e+00 -1.0198000e-02 /
CHEB / -2.9829000e+00 3.4627000e-01 6.4832000e-02 /
CHEB / -1.7032000e+00 -7.9743000e-02 3.7138000e-02 /
CHEB / -7.9508000e-01 -1.5398000e-01 -8.7406000e-03 /

OH+iC4H8(+m)=acetone+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -22.42757204710079
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3770000e+00 -6.4609000e-01 -1.8749000e-01 /
CHEB / 5.6858000e+00 7.3579000e-01 1.7893000e-01 /
CHEB / 2.1902000e-01 3.2391000e-02 5.3046000e-02 /
CHEB / -5.3850000e-02 -1.0778000e-01 -2.3522000e-02 /
CHEB / -6.2181000e-02 -3.9381000e-02 -2.6084000e-02 /

OH+iC4H8(+m)=H2CCCH3[OH]+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -10.659153777589246
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1170000e+01 -9.3181000e-01 -1.0830000e-01 /
CHEB / 1.4691000e+00 1.0507000e+00 5.6907000e-02 /
CHEB / -1.8625000e-01 6.2156000e-02 9.0536000e-02 /
CHEB / -1.5161000e-01 -1.5379000e-01 -6.0796000e-03 /
CHEB / -2.9113000e-02 -6.6055000e-02 -3.3086000e-02 /

H2CCCH3[OH]+CH3(+m)=OC[CH3]3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -18.947544143077153
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2745000e+01 5.3801000e+00 2.7484000e-01 /
CHEB / 6.8799000e+00 9.4370000e-02 1.1120000e-01 /
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CHEB / -1.6596000e+00 -4.0380000e-01 1.3311000e-01 /
CHEB / -1.0883000e+00 -2.2654000e-01 1.2958000e-02 /
CHEB / -6.2413000e-01 1.0756000e-02 -4.8946000e-02 /

H2CCCH3[OH]+CH3(+m)=HOC[CH2][CH3]2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (OC[CH3]3) High-P Limit: R_Addition_MultipleBond
exact:  Cd/Nd2_Cd/H2     C_methyl         deltaHrxn(T=298K) = -
20.547829809264673 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1403000e+00 7.7577000e-01 -5.5027000e-02 /
CHEB / -6.0313000e-01 1.0890000e+00 -1.0198000e-02 /
CHEB / -2.9671000e+00 3.4627000e-01 6.4832000e-02 /
CHEB / -1.6732000e+00 -7.9743000e-02 3.7138000e-02 /
CHEB / -7.7452000e-01 -1.5398000e-01 -8.7406000e-03 /

H2CCCH3[OH]+CH3(+m)=acetone+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -11.768418269511542
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3361000e-01 -6.4609000e-01 -1.8749000e-01 /
CHEB / 9.3978000e+00 7.3579000e-01 1.7893000e-01 /
CHEB / 2.3481000e-01 3.2391000e-02 5.3046000e-02 /
CHEB / -2.3843000e-02 -1.0778000e-01 -2.3522000e-02 /
CHEB / -4.1629000e-02 -3.9381000e-02 -2.6084000e-02 /

O+tC4H9(+m)=OC[CH3]3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3) High-P Limit: Oa_R_Recombination estimate:
(Average:) Oa     C_rad/Cs3         deltaHrxn(T=298K) = -
97.07007749786331 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0966000e+01 7.3412000e+00 2.5305000e+00 /
CHEB / -4.7796000e-01 3.9924000e+00 5.2777000e-01 /
CHEB / -1.4249000e+00 4.1892000e-01 -6.4246000e-01 /
CHEB / -9.3838000e-01 -2.4165000e-01 -4.3286000e-01 /
CHEB / -4.1708000e-01 -1.2160000e-01 -2.2762000e-01 /

O+tC4H9(+m)=HOC[CH2][CH3]2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -98.67036316405084
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2027000e+01 1.2844000e+01 1.1377000e+00 /
CHEB / -5.0410000e-01 -1.5466000e+00 -5.6338000e-01 /
CHEB / -1.6182000e+00 -1.4555000e+00 5.7996000e-02 /
CHEB / -1.2348000e+00 -6.8236000e-01 2.0941000e-01 /
CHEB / -8.2567000e-01 -1.3369000e-01 1.5858000e-01 /

O+tC4H9(+m)=acetone+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -89.89095162429771
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2994000e+01 1.1069000e-06 7.7052000e-07 /
CHEB / -3.4023000e-01 2.1376000e-06 1.4880000e-06 /
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CHEB / -2.1726000e-01 1.4139000e-06 9.8420000e-07 /
CHEB / -1.6951000e-01 4.7336000e-07 3.2952000e-07 /
CHEB / -1.3193000e-01 -2.4140000e-07 -1.6802000e-07 /

O+tC4H9(+m)=OH+iC4H8(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -67.46337957719692
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8806000e+00 -3.3227000e-05 -2.3139000e-05 /
CHEB / 1.8507000e+00 1.1240000e-05 7.8323000e-06 /
CHEB / 4.7094000e-01 2.0213000e-05 1.4075000e-05 /
CHEB / 7.5805000e-02 6.7930000e-06 4.7259000e-06 /
CHEB / -4.6401000e-02 -1.3502000e-06 -9.4256000e-07 /

O+tC4H9(+m)=H2CCCH3[OH]+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OC[CH3]3)     deltaHrxn(T=298K) = -78.12253335478616
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0298000e+01 -3.3227000e-05 -2.3139000e-05 /
CHEB / 2.1104000e+00 1.1240000e-05 7.8323000e-06 /
CHEB / 5.3920000e-01 2.0213000e-05 1.4075000e-05 /
CHEB / 9.9718000e-02 6.7930000e-06 4.7259000e-06 /
CHEB / -3.6989000e-02 -1.3502000e-06 -9.4256000e-07 /

!PDepNetwork C3H7O-N1 + C3H7O-N2 + HOCHC2H5 + OCH2CH2CH3
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     OCH2CH2CH3        -7.25 106.11      21.2  25.72 29.85 33.41 39.13
      43.44 50.19
!     C3H7O-N2          -13.23      80.42 21.04 25.11 28.98 32.38 37.87
      42.05 48.76
!     HOCHC2H5          -17.02      78.74 21.22 25.67 29.69 33.11 38.51
      42.57 49.06
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     C3H6O             -43.67      73.5  18.92 22.42 25.99 29.23 34.57
      38.63 44.94
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
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!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H6O-enol        -34.7 70.85 20.67 24.56 28.02 30.98 35.68 39.25
      45.02
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+CH2OH=C3H7O-N1     2.4100000e+10      0.00000
6.9600000e+03
!     C3H6O-enol2+H=C3H7O-N1        1.1800000e+13      0.00000
3.8000000e+03
!     OCH2CH2CH3=C3H7O-N1           9.0000000e+11      0.00000
2.9400000e+04
!     C2H5+CH2O=OCH2CH2CH3    7.9400000e+10      0.00000
6.7000000e+03
!     C3H6O+H=OCH2CH2CH3      1.0000000e+11      0.00000
1.1900000e+04
!     OCH2CH2CH3=C3H7O-N2           9.7200000e+09      1.17000
3.9660000e+04
!     C3H6O-enol2+H=C3H7O-N2        2.0100000e+13      0.00000
2.1000000e+03
!     C3H6+OH=C3H7O-N2        2.7100000e+12      0.00000
0.0000000e+00
!     C3H6O-enol+H=C3H7O-N2         1.0000000e+13      0.00000
2.9000000e+03
!     C3H7O-N1=C3H7O-N2             3.8760000e+10      0.89000
3.5800000e+04
!     C3H7O-N2=HOCHC2H5             1.3103945e+11      0.63800
3.9880000e+04
!     C3H6O+H=HOCHC2H5        2.3501400e+11      0.30815
4.9629937e+03
!     CH3+C2H4O=HOCHC2H5      3.1000000e+12      0.00000
8.5000000e+03
!     C3H6O-enol+H=HOCHC2H5         1.0000000e+13      0.00000
2.9000000e+03
!     C3H7O-N1=HOCHC2H5             2.1620731e+09      0.93000
3.2050000e+04
!     OCH2CH2CH3=HOCHC2H5           8.1282219e+08      1.13906
3.4790987e+04
!     C3H7-1+O=OCH2CH2CH3     1.0000000e+13      0.00000
0.0000000e+00

C3H7O-N1(+m)=OCH2CH2CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = 3.719753581487126
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2991000e-02 1.4513000e+00 -1.4338000e-01 /
CHEB / 5.0128000e+00 1.1499000e+00 1.7625000e-01 /
CHEB / -3.7530000e+00 1.7165000e-01 9.3767000e-02 /
CHEB / -2.0051000e+00 -7.2138000e-02 1.4752000e-02 /
CHEB / -9.8455000e-01 -1.2714000e-01 2.6524000e-02 /
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C3H7O-N1(+m)=C3H7O-N2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.259633419168537 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5322000e+00 2.7172000e+00 -5.8525000e-01 /
CHEB / 6.4139000e+00 9.6985000e-01 1.5915000e-01 /
CHEB / -3.4334000e+00 2.1092000e-02 8.6073000e-02 /
CHEB / -2.1342000e+00 -2.9570000e-02 1.1501000e-01 /
CHEB / -1.2238000e+00 -1.2067000e-01 9.2429000e-02 /

C3H7O-N1(+m)=HOCHC2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -6.049255111825493 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9542000e+00 1.6222000e+00 -1.9114000e-01 /
CHEB / 5.6055000e+00 1.2687000e+00 1.2681000e-01 /
CHEB / -3.3559000e+00 7.6081000e-02 1.5155000e-01 /
CHEB / -1.9642000e+00 -2.7788000e-01 1.5755000e-01 /
CHEB / -1.0781000e+00 -3.1921000e-01 1.4325000e-01 /

OCH2CH2CH3(+m)=HOCHC2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    O_rad_out     Cs_H_out_H/(NonDeC/Cs)
      deltaHrxn(T=298K) = -9.76900869331262 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3100000e+00 2.1404000e+00 -4.8920000e-01 /
CHEB / 6.3108000e+00 1.1362000e+00 1.4882000e-01 /
CHEB / -3.7916000e+00 1.8139000e-01 1.8543000e-01 /
CHEB / -2.3027000e+00 -5.2255000e-02 3.9154000e-02 /
CHEB / -1.1658000e+00 -1.8384000e-01 4.2962000e-02 /

C3H7O-N2(+m)=OCH2CH2CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = 5.979387000655663
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.4804000e+00 2.2806000e+00 -5.2589000e-01 /
CHEB / 9.3856000e+00 1.5564000e+00 -3.4418000e-03 /
CHEB / -3.8006000e+00 -9.4742000e-02 2.4801000e-01 /
CHEB / -2.3519000e+00 -6.0280000e-02 9.0046000e-02 /
CHEB / -1.1563000e+00 -1.4716000e-01 2.2626000e-02 /

C3H7O-N2(+m)=HOCHC2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_H/NonDeC     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -3.789621692656956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0732000e+00 3.1937000e+00 -9.7359000e-01 /
CHEB / 8.2231000e+00 1.1150000e+00 2.1586000e-01 /
CHEB / -3.5379000e+00 4.0428000e-02 1.9990000e-01 /
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CHEB / -2.1802000e+00 -2.3496000e-01 1.3123000e-01 /
CHEB / -1.2051000e+00 -2.2112000e-01 8.0150000e-02 /

C2H4+CH2OH(+m)=C3H7O-N1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H2     C_rad/H2/O          deltaHrxn(T=298K) = -
20.67800168083977 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1513000e+00 6.1961000e-01 1.5255000e-02 /
CHEB / -1.5127000e+00 8.4198000e-01 1.3872000e-02 /
CHEB / -2.2367000e+00 3.4034000e-01 -5.3980000e-02 /
CHEB / -9.7673000e-01 1.5481000e-01 -5.6513000e-02 /
CHEB / -3.8093000e-01 1.0234000e-01 1.8402000e-02 /

C2H4+CH2OH(+m)=OCH2CH2CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -16.958248099352645
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0597000e+00 -7.0177000e-02 -1.8101000e-01 /
CHEB / 1.9593000e+00 1.5662000e+00 8.2158000e-02 /
CHEB / -1.5654000e+00 4.4239000e-01 -2.3508000e-02 /
CHEB / -9.4731000e-01 2.4703000e-01 -1.4714000e-02 /
CHEB / -5.9428000e-01 1.0955000e-01 5.9153000e-02 /

C2H4+CH2OH(+m)=C3H7O-N2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -22.937635100008308
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7993000e-01 1.0322000e+00 -6.3591000e-01 /
CHEB / 3.0212000e+00 1.4429000e+00 2.5061000e-02 /
CHEB / -1.5962000e+00 3.1526000e-01 5.7732000e-02 /
CHEB / -1.1237000e+00 1.8103000e-01 6.8169000e-02 /
CHEB / -6.3965000e-01 3.6364000e-02 4.5502000e-02 /

C2H4+CH2OH(+m)=HOCHC2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -26.727256792665266
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0387000e+00 4.6563000e-01 -4.4259000e-01 /
CHEB / 2.5590000e+00 1.7727000e+00 -5.3879000e-02 /
CHEB / -1.4441000e+00 3.3669000e-01 6.6565000e-02 /
CHEB / -1.0953000e+00 1.4684000e-01 4.8863000e-02 /
CHEB / -6.7699000e-01 7.1877000e-02 3.4926000e-02 /

C2H4+CH2OH(+m)=C2H5+CH2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -6.499252225847105
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7864000e+00 -1.9881000e+00 -1.7131000e-01 /
CHEB / 4.5373000e+00 1.4775000e+00 8.5660000e-02 /
CHEB / 2.2401000e-01 3.8012000e-01 -3.0446000e-02 /
CHEB / 8.9954000e-02 2.5469000e-01 3.8286000e-03 /
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CHEB / -7.0214000e-02 1.1052000e-01 7.2706000e-02 /

C2H4+CH2OH(+m)=CH3+C2H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -3.580041116106056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2893000e+00 -1.8577000e+00 -2.3144000e-01 /
CHEB / 6.6257000e+00 1.2574000e+00 1.3550000e-01 /
CHEB / 1.2318000e-01 5.1821000e-01 -1.4140000e-02 /
CHEB / -8.7465000e-02 2.0087000e-01 2.4836000e-02 /
CHEB / 2.1075000e-02 4.7712000e-02 5.2705000e-02 /

C3H6O-enol2+H(+m)=C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/Nd_Cd/H2     H_rad       deltaHrxn(T=298K) = -34.135874146465476
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0407000e+00 1.6901000e+00 -9.1779000e-02 /
CHEB / -1.8018000e+00 -1.8528000e-01 1.0984000e-01 /
CHEB / -1.3513000e+00 2.8058000e-01 -3.1834000e-01 /
CHEB / -7.4490000e-01 5.9254000e-01 -2.4404000e-02 /
CHEB / -5.2715000e-01 2.7313000e-01 1.9072000e-01 /

C3H6O-enol2+H(+m)=OCH2CH2CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -30.41612056497835
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0949000e+01 3.1777000e-01 -1.9744000e-01 /
CHEB / 2.7707000e-01 1.2347000e+00 3.0770000e-02 /
CHEB / -1.3531000e+00 5.9278000e-01 -6.0418000e-02 /
CHEB / -1.0384000e+00 3.4258000e-01 3.3571000e-02 /
CHEB / -6.3387000e-01 6.1300000e-02 6.0035000e-02 /

C3H6O-enol2+H(+m)=C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H/Nd     H_rad       deltaHrxn(T=298K) = -36.39550756563401
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7577000e+00 1.4985000e+00 -4.5946000e-01 /
CHEB / -3.0225000e+00 1.0672000e+00 -6.5675000e-02 /
CHEB / -2.2580000e+00 3.1818000e-01 1.7011000e-02 /
CHEB / -1.0841000e+00 7.9790000e-02 1.2050000e-02 /
CHEB / -4.3253000e-01 4.5787000e-02 3.2376000e-02 /

C3H6O-enol2+H(+m)=HOCHC2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -40.18512925829097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1467000e+00 1.0906000e+00 -6.2738000e-01 /
CHEB / 7.5458000e-01 1.1950000e+00 1.2474000e-01 /
CHEB / -1.4674000e+00 4.6209000e-01 1.3874000e-02 /
CHEB / -1.0940000e+00 2.2968000e-01 1.2694000e-02 /
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CHEB / -6.1922000e-01 7.8710000e-02 5.1588000e-02 /

C3H6O-enol2+H(+m)=C2H4+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -13.457872465625705
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9072000e+00 -5.6851000e-01 -7.2679000e-02 /
CHEB / 1.4453000e+00 -8.9459000e-03 8.3287000e-02 /
CHEB / 4.2245000e-01 1.9488000e-01 -1.7132000e-01 /
CHEB / 2.2728000e-01 4.0118000e-01 1.0163000e-03 /
CHEB / 4.4663000e-02 1.7191000e-01 1.2364000e-01 /

C3H6O-enol2+H(+m)=C2H5+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -19.95712469147281
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0243000e+00 -1.7058000e+00 -1.7431000e-01 /
CHEB / 2.6675000e+00 1.1496000e+00 5.4318000e-02 /
CHEB / 3.1732000e-01 5.1162000e-01 -2.5270000e-02 /
CHEB / 8.4705000e-03 2.7454000e-01 5.4238000e-02 /
CHEB / -4.1986000e-02 3.9525000e-02 6.2144000e-02 /

C3H6O-enol2+H(+m)=C3H6O+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -14.738144775732785
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4365000e+00 -1.7443000e+00 -2.3166000e-01 /
CHEB / 4.2895000e+00 1.1559000e+00 1.1576000e-01 /
CHEB / 1.6024000e-01 5.1677000e-01 5.9275000e-03 /
CHEB / -1.6189000e-02 1.8427000e-01 2.8972000e-02 /
CHEB / 8.1806000e-02 5.1494000e-02 5.5317000e-02 /

C3H6O-enol2+H(+m)=C3H6+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -8.23851538412369
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1396000e+01 -8.8353000e-01 -2.0054000e-01 /
CHEB / 6.7020000e-01 6.3969000e-01 1.2006000e-01 /
CHEB / -8.5734000e-02 6.8970000e-02 2.8886000e-02 /
CHEB / 2.2108000e-01 4.5274000e-02 -4.0400000e-02 /
CHEB / 2.3762000e-01 1.2368000e-01 3.8227000e-03 /

C3H6O-enol2+H(+m)=C3H6O-enol+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -5.769265895614019
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1696000e+00 -8.9642000e-01 -1.9016000e-01 /
CHEB / 2.0967000e+00 5.7494000e-01 1.2568000e-01 /
CHEB / 3.4477000e-01 6.4939000e-02 1.3944000e-02 /
CHEB / 3.5884000e-01 1.1838000e-01 -5.1557000e-02 /
CHEB / 2.4363000e-01 1.8708000e-01 8.4905000e-03 /
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C3H6O-enol2+H(+m)=CH3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -17.03791358173176
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1970000e+00 -1.7459000e+00 -2.3032000e-01 /
CHEB / 4.1085000e+00 1.1589000e+00 1.1305000e-01 /
CHEB / 1.0481000e-01 5.0619000e-01 7.3787000e-03 /
CHEB / -2.8639000e-02 1.7895000e-01 3.0304000e-02 /
CHEB / 7.8377000e-02 5.3868000e-02 5.5652000e-02 /

C2H5+CH2O(+m)=C3H7O-N1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -14.178749454992667
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2729000e+00 -2.8646000e-01 -1.6099000e-01 /
CHEB / 3.1869000e+00 1.4700000e+00 1.3190000e-01 /
CHEB / -1.7910000e+00 3.9835000e-01 3.7312000e-02 /
CHEB / -9.6449000e-01 1.5448000e-01 -4.5354000e-03 /
CHEB / -5.7927000e-01 5.5973000e-02 4.2028000e-02 /

C2H5+CH2O(+m)=OCH2CH2CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond exact:
C_rad/H2/Cs     CO/H2_O       deltaHrxn(T=298K) = -10.458995873505541
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5494000e+00 3.5790000e-01 -1.5419000e-02 /
CHEB / 8.9138000e-01 6.5232000e-01 -2.0666000e-02 /
CHEB / -1.1308000e+00 4.8350000e-01 4.7029000e-03 /
CHEB / -8.6766000e-01 2.6391000e-01 3.3513000e-02 /
CHEB / -6.0975000e-01 5.8978000e-02 5.3908000e-02 /

C2H5+CH2O(+m)=C3H7O-N2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -16.438382874161206
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7291000e+00 6.1231000e-01 -5.8966000e-01 /
CHEB / 6.4351000e+00 1.6509000e+00 -5.0360000e-03 /
CHEB / -2.0521000e+00 1.3974000e-01 2.1063000e-01 /
CHEB / -1.2794000e+00 1.3209000e-01 2.8730000e-02 /
CHEB / -6.3837000e-01 -1.8237000e-02 2.8011000e-02 /

C2H5+CH2O(+m)=HOCHC2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -20.22800456681816
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1918000e-01 4.2022000e-01 -5.3718000e-01 /
CHEB / 5.5860000e+00 1.3834000e+00 1.4275000e-01 /
CHEB / -1.9087000e+00 4.0470000e-01 1.1487000e-01 /
CHEB / -1.2140000e+00 1.1475000e-01 1.7219000e-02 /
CHEB / -6.8087000e-01 -1.8370000e-02 4.2895000e-02 /
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C3H6O+H(+m)=C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -19.397729370732698
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7457000e+00 -9.0306000e-02 -2.0953000e-01 /
CHEB / 3.1672000e+00 1.4556000e+00 1.0339000e-01 /
CHEB / -1.5929000e+00 4.8639000e-01 2.4368000e-02 /
CHEB / -1.1993000e+00 2.7918000e-01 -4.3631000e-04 /
CHEB / -6.7279000e-01 6.2125000e-02 3.8213000e-02 /

C3H6O+H(+m)=OCH2CH2CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H/Nd_O     H_rad        deltaHrxn(T=298K) = -
15.67797578924557 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8342000e+00 2.5945000e-01 -1.0385000e-01 /
CHEB / 3.8291000e+00 8.5156000e-01 -6.3076000e-02 /
CHEB / -1.5269000e+00 8.3119000e-01 8.7611000e-02 /
CHEB / -1.3796000e+00 2.3331000e-01 2.7262000e-02 /
CHEB / -6.5868000e-01 -3.7329000e-02 -6.3650000e-03 /

C3H6O+H(+m)=C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -21.657362789901235
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4754000e+00 9.9046000e-01 -7.4862000e-01 /
CHEB / 4.4032000e+00 1.3759000e+00 1.6747000e-01 /
CHEB / -1.8503000e+00 3.6841000e-01 9.6107000e-02 /
CHEB / -1.2632000e+00 1.3817000e-01 2.8323000e-02 /
CHEB / -6.6325000e-01 2.3220000e-02 3.7893000e-02 /

C3H6O+H(+m)=HOCHC2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
25.44698448255819 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5279000e+00 5.2760000e-01 -4.8174000e-02 /
CHEB / -1.6108000e+00 7.7768000e-01 -2.6897000e-02 /
CHEB / -2.2373000e+00 3.0496000e-01 5.3623000e-02 /
CHEB / -1.2532000e+00 3.4602000e-02 6.3186000e-02 /
CHEB / -5.5841000e-01 -7.5200000e-03 4.3326000e-02 /

C3H6O+H(+m)=C2H4+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = 1.2802723101070757
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9644000e+00 -1.8690000e+00 -2.3276000e-01 /
CHEB / 6.8868000e+00 1.2693000e+00 1.3771000e-01 /
CHEB / 4.3575000e-02 5.1207000e-01 -1.2230000e-02 /
CHEB / -1.4181000e-01 2.1619000e-01 1.9781000e-02 /
CHEB / -2.1578000e-03 4.2471000e-02 5.3640000e-02 /
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C3H6O+H(+m)=C2H5+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -5.218979915740029
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5730000e+00 -1.7696000e+00 -1.2198000e-01 /
CHEB / 6.4687000e+00 9.6205000e-01 -4.4071000e-02 /
CHEB / 4.9982000e-02 7.8951000e-01 9.8217000e-02 /
CHEB / -2.8877000e-01 1.4647000e-01 -5.9006000e-03 /
CHEB / -5.8334000e-02 2.8619000e-02 1.0241000e-02 /

C3H6O+H(+m)=CH3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -2.29976880599898
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8569000e+00 -1.1094000e+00 -1.2121000e-01 /
CHEB / 3.1711000e+00 9.2009000e-01 -6.5951000e-03 /
CHEB / -1.3167000e-01 1.0379000e-01 5.5473000e-02 /
CHEB / 3.9952000e-02 -4.2191000e-02 -3.0426000e-03 /
CHEB / 1.4514000e-01 6.2393000e-02 6.0914000e-03 /

C3H6+OH(+m)=C3H7O-N1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -25.89735876234179
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6783000e+00 3.7096000e-01 -2.8723000e-01 /
CHEB / 1.7086000e+00 8.5353000e-01 2.3969000e-01 /
CHEB / -1.7456000e+00 6.5647000e-01 -9.7638000e-02 /
CHEB / -1.2295000e+00 3.5009000e-01 4.7018000e-02 /
CHEB / -6.2089000e-01 -1.5273000e-02 6.4326000e-02 /

C3H6+OH(+m)=OCH2CH2CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -22.177605180854663
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2381000e+00 -5.8263000e-02 -2.5176000e-01 /
CHEB / 3.2537000e+00 1.4452000e+00 1.3595000e-01 /
CHEB / -2.1751000e+00 5.5140000e-01 3.1173000e-02 /
CHEB / -1.2556000e+00 2.3055000e-01 -1.4898000e-02 /
CHEB / -6.0283000e-01 4.4255000e-02 3.7971000e-02 /

C3H6+OH(+m)=C3H7O-N2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/Nd     O_pri_rad      deltaHrxn(T=298K)
= -28.156992181510326 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0636000e+01 4.8066000e-01 -8.1214000e-02 /
CHEB / -3.3591000e+00 6.7268000e-01 -6.3497000e-02 /
CHEB / -2.3064000e+00 2.2269000e-01 4.9630000e-02 /
CHEB / -1.2941000e+00 -1.1737000e-02 7.5175000e-02 /
CHEB / -5.7618000e-01 -2.6540000e-02 5.4628000e-02 /
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C3H6+OH(+m)=HOCHC2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -31.94661387416728
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3131000e+00 9.8198000e-01 -7.0960000e-01 /
CHEB / 2.3828000e+00 1.0743000e+00 2.9156000e-01 /
CHEB / -1.7591000e+00 3.9830000e-01 4.7870000e-02 /
CHEB / -1.2943000e+00 2.5131000e-01 -1.5801000e-02 /
CHEB / -6.8824000e-01 5.0585000e-02 4.8974000e-02 /

C3H6+OH(+m)=C2H4+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -5.2193570815020145
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3552000e+00 -1.6726000e+00 -2.3880000e-01 /
CHEB / 4.9293000e+00 9.8541000e-01 1.5799000e-01 /
CHEB / -9.6309000e-02 6.1330000e-01 -4.8791000e-02 /
CHEB / -1.0261000e-01 2.0560000e-01 5.5739000e-02 /
CHEB / 3.6464000e-02 2.5538000e-02 4.1776000e-02 /

C3H6+OH(+m)=C2H5+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -11.71860930734912
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3675000e+00 -2.0000000e+00 -2.4621000e-01 /
CHEB / 5.3973000e+00 1.4018000e+00 1.4548000e-01 /
CHEB / -4.8254000e-01 5.2163000e-01 1.6316000e-02 /
CHEB / -1.4161000e-01 2.0211000e-01 -8.4786000e-03 /
CHEB / -2.6592000e-02 6.4834000e-02 4.5210000e-02 /

C3H6+OH(+m)=C3H6O+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7O-N1)     deltaHrxn(T=298K) = -6.499629391609091 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3561000e+00 -1.7057000e+00 -3.2461000e-01 /
CHEB / 5.9558000e+00 1.0112000e+00 2.6673000e-01 /
CHEB / -1.3953000e-01 6.1563000e-01 -4.8835000e-02 /
CHEB / -1.8273000e-01 2.2692000e-01 1.7919000e-02 /
CHEB / 4.7279000e-02 1.3238000e-02 5.7017000e-02 /

C3H6+OH(+m)=CH3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -8.79939819760807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0982000e+00 -1.7032000e+00 -3.1962000e-01 /
CHEB / 5.7787000e+00 1.0154000e+00 2.5931000e-01 /
CHEB / -1.9209000e-01 6.1279000e-01 -4.9032000e-02 /
CHEB / -1.8886000e-01 2.1745000e-01 2.2292000e-02 /
CHEB / 4.7171000e-02 1.5292000e-02 5.6417000e-02 /

C3H6O-enol+H(+m)=C3H7O-N1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -28.366608250851456
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4692000e+00 1.2461000e-01 -2.3485000e-01 /
CHEB / 1.2226000e+00 1.3145000e+00 1.1088000e-01 /
CHEB / -1.5353000e+00 5.8276000e-01 -3.0555000e-02 /
CHEB / -1.1371000e+00 3.0759000e-01 1.0627000e-02 /
CHEB / -5.9334000e-01 3.4023000e-02 5.0289000e-02 /

C3H6O-enol+H(+m)=OCH2CH2CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -24.64685466936433
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3035000e+00 -3.4362000e-02 -2.4763000e-01 /
CHEB / 2.3393000e+00 1.5109000e+00 1.1116000e-01 /
CHEB / -1.7808000e+00 5.9599000e-01 3.7950000e-03 /
CHEB / -1.1771000e+00 2.2517000e-01 -1.1075000e-02 /
CHEB / -5.9999000e-01 6.3084000e-02 3.9402000e-02 /

C3H6O-enol+H(+m)=C3H7O-N2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/Nd     H_rad        deltaHrxn(T=298K)
= -30.626241670019994 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6970000e+00 8.6418000e-01 -1.9412000e-01 /
CHEB / -2.5619000e+00 1.0001000e+00 -8.4938000e-02 /
CHEB / -2.2977000e+00 3.3842000e-01 5.7036000e-02 /
CHEB / -1.2029000e+00 6.3475000e-02 6.4002000e-02 /
CHEB / -5.0652000e-01 2.6794000e-02 4.6463000e-02 /

C3H6O-enol+H(+m)=HOCHC2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/Nd     H_rad        deltaHrxn(T=298K)
= -34.415863362676944 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7355000e+00 1.1199000e+00 -2.7653000e-01 /
CHEB / -2.6773000e+00 1.1494000e+00 -1.2944000e-01 /
CHEB / -2.1403000e+00 3.4363000e-01 -4.2547000e-03 /
CHEB / -1.0638000e+00 5.1340000e-02 6.9814000e-03 /
CHEB / -4.6177000e-01 1.5325000e-02 3.3888000e-02 /

C3H6O-enol+H(+m)=C2H4+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -7.688606570011682
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0642000e+00 -1.7953000e+00 -2.1471000e-01 /
CHEB / 4.6891000e+00 1.1920000e+00 1.0829000e-01 /
CHEB / 7.0623000e-02 5.2295000e-01 -1.0254000e-02 /
CHEB / -4.3536000e-02 1.8226000e-01 3.8234000e-02 /
CHEB / 4.5743000e-02 5.4950000e-02 4.9031000e-02 /

C3H6O-enol+H(+m)=C2H5+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -14.187858795858787
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3437000e+00 -1.9938000e+00 -2.3333000e-01 /
CHEB / 4.6651000e+00 1.4451000e+00 1.2555000e-01 /
CHEB / -9.6736000e-02 5.1195000e-01 8.2449000e-03 /
CHEB / -9.8894000e-02 1.9634000e-01 1.3891000e-03 /
CHEB / -1.5400000e-02 6.7087000e-02 5.1210000e-02 /

C3H6O-enol+H(+m)=C3H6O+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -8.968878880118758
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5966000e+00 -9.5875000e-01 -1.5793000e-01 /
CHEB / 1.6488000e+00 7.5816000e-01 7.7958000e-02 /
CHEB / 1.1471000e-01 3.9513000e-02 3.5467000e-02 /
CHEB / 1.9224000e-01 2.0912000e-02 -4.9077000e-02 /
CHEB / 1.7446000e-01 1.2709000e-01 -8.9524000e-03 /

C3H6O-enol+H(+m)=C3H6+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -2.469249488509668
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0590000e+01 -1.0850000e+00 -1.5877000e-01 /
CHEB / 1.4282000e+00 8.2607000e-01 2.3598000e-02 /
CHEB / -1.3167000e-01 1.3138000e-01 6.3292000e-02 /
CHEB / 9.4268000e-02 2.5644000e-02 -2.3046000e-04 /
CHEB / 1.8723000e-01 8.8649000e-02 1.0504000e-02 /

C3H6O-enol+H(+m)=CH3+C2H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -11.268647686117738
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1228000e+01 -9.3806000e-01 -1.5830000e-01 /
CHEB / 1.5783000e+00 7.3179000e-01 8.7307000e-02 /
CHEB / 8.7838000e-02 2.3686000e-02 2.9940000e-02 /
CHEB / 1.8172000e-01 3.4380000e-02 -5.6277000e-02 /
CHEB / 1.6635000e-01 1.4275000e-01 -9.3549000e-03 /

CH3+C2H4O(+m)=C3H7O-N1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -17.097960564733718
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7451000e+00 -4.6278000e-02 -2.1764000e-01 /
CHEB / 3.9306000e+00 1.4405000e+00 1.0450000e-01 /
CHEB / -1.5783000e+00 5.0786000e-01 1.4097000e-02 /
CHEB / -1.1671000e+00 2.9215000e-01 -4.0001000e-03 /
CHEB / -6.3596000e-01 5.4642000e-02 4.1487000e-02 /

CH3+C2H4O(+m)=OCH2CH2CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -13.37820698324659
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 5.4241000e+00 -9.2058000e-02 -2.4447000e-01 /
CHEB / 5.2917000e+00 1.4562000e+00 1.3514000e-01 /
CHEB / -1.9301000e+00 5.9966000e-01 1.9040000e-02 /
CHEB / -1.2042000e+00 2.1748000e-01 -9.7100000e-03 /
CHEB / -6.1728000e-01 4.9468000e-02 3.2765000e-02 /

CH3+C2H4O(+m)=C3H7O-N2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -19.357593983902255
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5101000e-01 1.0185000e+00 -7.5172000e-01 /
CHEB / 5.0696000e+00 1.3913000e+00 1.6034000e-01 /
CHEB / -1.8215000e+00 3.7179000e-01 9.0157000e-02 /
CHEB / -1.2209000e+00 1.4795000e-01 2.4732000e-02 /
CHEB / -6.3281000e-01 2.7505000e-02 3.8987000e-02 /

CH3+C2H4O(+m)=HOCHC2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: R_Addition_MultipleBond exact:
C_methyl     Cd/H2_Cd/H/Nd          deltaHrxn(T=298K) = -
23.14721567655921 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0837000e+00 6.6237000e-01 -8.8898000e-02 /
CHEB / -5.5820000e-01 9.1952000e-01 -5.7481000e-02 /
CHEB / -2.2820000e+00 3.3911000e-01 4.5534000e-02 /
CHEB / -1.2085000e+00 4.9230000e-02 5.2774000e-02 /
CHEB / -5.2102000e-01 8.2285000e-03 3.8299000e-02 /

CH3+C2H4O(+m)=C2H5+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -2.919211109741049
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3885000e+00 -2.0329000e+00 -2.3579000e-01 /
CHEB / 7.6122000e+00 1.4292000e+00 1.3716000e-01 /
CHEB / -2.0732000e-01 5.3597000e-01 1.0532000e-02 /
CHEB / -1.2598000e-01 2.0097000e-01 -4.3268000e-03 /
CHEB / -4.6456000e-02 6.3983000e-02 4.3485000e-02 /

C3H7-1+O(+m)=C3H7O-N1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -95.81031834270561
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7071000e+00 5.7457000e+00 -2.2082000e+00 /
CHEB / -8.6591000e-01 -1.2391000e+00 8.0033000e-01 /
CHEB / -5.7046000e-01 -4.0985000e-01 4.6458000e-01 /
CHEB / -8.1917000e-01 2.5664000e-01 1.5488000e-01 /
CHEB / -7.3835000e-01 2.4099000e-01 4.1430000e-02 /

C3H7-1+O(+m)=OCH2CH2CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1) High-P Limit: Oa_R_Recombination estimate:
(Average:) C_rad/H2/Cs     Oa       deltaHrxn(T=298K) = -
92.09056476121849 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 8.8159000e+00 5.6992000e+00 -2.2193000e+00 /
CHEB / -1.9250000e-01 -1.1843000e+00 8.1309000e-01 /
CHEB / -5.9465000e-01 -4.0593000e-01 4.6748000e-01 /
CHEB / -9.1022000e-01 2.4779000e-01 1.5230000e-01 /
CHEB / -7.5206000e-01 2.3216000e-01 3.8013000e-02 /

C3H7-1+O(+m)=C3H7O-N2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -98.06995176187415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1192000e+00 7.2412000e+00 -2.7349000e+00 /
CHEB / -5.0262000e-01 -1.8429000e+00 8.6291000e-01 /
CHEB / -6.9570000e-01 -4.9004000e-01 5.2322000e-01 /
CHEB / -8.2988000e-01 2.1643000e-01 1.7531000e-01 /
CHEB / -7.0551000e-01 1.8981000e-01 5.3260000e-02 /

C3H7-1+O(+m)=HOCHC2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -101.8595734545311
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2877000e+00 6.8115000e+00 -2.5567000e+00 /
CHEB / -7.2792000e-02 -1.6405000e+00 8.1878000e-01 /
CHEB / -6.7221000e-01 -5.4433000e-01 4.9450000e-01 /
CHEB / -8.8971000e-01 2.5250000e-01 1.7496000e-01 /
CHEB / -7.5271000e-01 2.4485000e-01 4.8515000e-02 /

C3H7-1+O(+m)=C2H4+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -75.13231666186583
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0723000e+01 -5.6481000e-01 -2.8806000e-01 /
CHEB / -4.5486000e-01 2.0073000e-01 1.0206000e-01 /
CHEB / 1.4207000e-01 1.6389000e-01 8.0781000e-02 /
CHEB / 1.0139000e-01 1.4415000e-01 6.7424000e-02 /
CHEB / 3.3867000e-02 9.1539000e-02 4.6730000e-02 /

C3H7-1+O(+m)=C3H6O-enol2+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -61.67444419624014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0673000e+01 -6.2771000e-01 -2.9693000e-01 /
CHEB / 5.9395000e-01 1.8972000e-01 9.3010000e-02 /
CHEB / 4.2932000e-01 1.4325000e-01 7.0826000e-02 /
CHEB / 2.2467000e-01 1.3415000e-01 6.0344000e-02 /
CHEB / 8.6706000e-02 9.3476000e-02 4.4282000e-02 /

C3H7-1+O(+m)=C2H5+CH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -81.63156888771294
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0679000e+01 -3.5473000e-01 -2.7057000e-01 /
CHEB / 1.6857000e-01 3.0654000e-01 1.1841000e-01 /
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CHEB / 3.0851000e-01 2.3970000e-01 9.9875000e-02 /
CHEB / 1.2497000e-01 1.6555000e-01 8.6185000e-02 /
CHEB / -1.2386000e-03 5.7576000e-02 5.6921000e-02 /

C3H7-1+O(+m)=C3H6O+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -76.41258897197292
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0604000e+01 -5.3698000e-01 -2.8484000e-01 /
CHEB / 5.3562000e-01 2.1629000e-01 1.0755000e-01 /
CHEB / 1.1536000e-01 1.7269000e-01 8.4714000e-02 /
CHEB / 1.2833000e-01 1.4676000e-01 7.0044000e-02 /
CHEB / 6.9692000e-02 8.7302000e-02 4.7293000e-02 /

C3H7-1+O(+m)=C3H6+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -69.91295958036383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1989000e+01 -5.5384000e-01 -2.8641000e-01 /
CHEB / -3.0834000e-01 2.1286000e-01 1.0490000e-01 /
CHEB / 1.3212000e-01 1.6506000e-01 8.2428000e-02 /
CHEB / 1.1813000e-01 1.4641000e-01 6.8919000e-02 /
CHEB / 3.7816000e-02 8.9538000e-02 4.6966000e-02 /

C3H7-1+O(+m)=C3H6O-enol+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -67.44371009185417
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0553000e+01 -5.9175000e-01 -2.9203000e-01 /
CHEB / 6.0740000e-01 1.9847000e-01 9.9295000e-02 /
CHEB / 3.0713000e-01 1.5380000e-01 7.6853000e-02 /
CHEB / 1.7826000e-01 1.4098000e-01 6.4812000e-02 /
CHEB / 8.3462000e-02 9.3200000e-02 4.5984000e-02 /

C3H7-1+O(+m)=CH3+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O-N1)     deltaHrxn(T=298K) = -78.7123577779719
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2551000e+01 -5.5523000e-01 -2.8730000e-01 /
CHEB / 2.2141000e-01 2.0866000e-01 1.0495000e-01 /
CHEB / 4.0575000e-02 1.6656000e-01 8.2235000e-02 /
CHEB / 1.0470000e-01 1.4473000e-01 6.8283000e-02 /
CHEB / 6.3062000e-02 8.9921000e-02 4.6933000e-02 /

!PDepNetwork C2H5O-1 C2H5O-2 C2H5O-3
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
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!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H5O-3           -2.66 66.84 15.8  18.82 21.65 24.13 28.15 31.21
      36.01
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+OH=C2H5O-1         2.7100000e+12      0.00000
0.0000000e+00
!     C2H4O+H=C2H5O-1         1.1800000e+13      0.00000
3.8000000e+03
!     C2H5O-1=C2H5O-2               4.6755363e+09      1.08500
3.1850000e+04
!     C2H4O+H=C2H5O-2         2.0100000e+13      0.00000
2.1000000e+03
!     CH3CHO+H=C2H5O-2        2.3501400e+11      0.30815
4.9629937e+03
!     C2H5O-3=C2H5O-2               8.1282219e+08      1.13906
3.4790987e+04
!     CH3+CH2O=C2H5O-3        3.1600000e+10      0.00000
1.1510000e+04
!     CH3CHO+H=C2H5O-3        1.0000000e+11      0.00000
1.1900000e+04
!     C2H5O-3=C2H5O-1               4.2390000e+09      1.45000
4.2270000e+04
!     C2H5+O=C2H5O-3          1.0000000e+13      0.00000
0.0000000e+00

C2H5O-1(+m)=C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -7.129118508814777 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2355000e+00 2.6186000e+00 -7.9342000e-01 /
CHEB / 8.2061000e+00 1.1350000e+00 1.3363000e-01 /
CHEB / -1.6571000e+00 2.4350000e-01 1.1857000e-01 /
CHEB / -9.2281000e-01 -7.1708000e-02 3.2926000e-02 /
CHEB / -4.6593000e-01 -1.2012000e-01 -1.1562000e-02 /

C2H5O-3(+m)=C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: intra_H_migration estimate: (Average:)
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```
Others-R3H_SS    O_rad_out     Cs_H_out_2H      deltaHrxn(T=298K) = -
3.129841845968783 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0314000e+01 5.9685000e+00 -1.1281000e+00 /
CHEB / 1.0973000e+01 7.1753000e-01 4.8576000e-01 /
CHEB / -1.4521000e+00 -1.0318000e-01 7.8316000e-02 /
CHEB / -9.2269000e-01 -1.9822000e-01 -3.4687000e-02 /
CHEB / -4.7080000e-01 -1.2191000e-01 -4.0135000e-02 /

C2H5O-3(+m)=C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    O_rad_out     Cs_H_out_H/NonDeC       deltaHrxn(T=298K)
= -10.25896035478356 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3969000e+00 6.2100000e+00 -1.2369000e+00 /
CHEB / 9.3368000e+00 6.7679000e-01 2.4425000e-01 /
CHEB / -1.6929000e+00 5.8716000e-02 1.7989000e-01 /
CHEB / -9.4525000e-01 -1.0884000e-01 2.4099000e-02 /
CHEB / -4.8194000e-01 -1.1185000e-01 -3.7118000e-02 /

C2H4+OH(+m)=C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H2
O_pri_rad         deltaHrxn(T=298K) = -28.027148280303585 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1100000e+01 8.5680000e-01 -1.3851000e-01 /
CHEB / -1.9142000e+00 7.6643000e-01 6.2856000e-02 /
CHEB / -1.2074000e+00 2.3621000e-01 7.1501000e-02 /
CHEB / -6.6981000e-01 3.0217000e-04 2.9791000e-02 /
CHEB / -3.4387000e-01 -5.6010000e-02 3.1016000e-04 /

C2H4+OH(+m)=C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -35.15626678911836 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1408000e+00 1.0142000e+00 -6.4893000e-01 /
CHEB / 8.6888000e-02 1.7386000e+00 2.0628000e-01 /
CHEB / -1.1723000e+00 3.6653000e-01 1.5566000e-01 /
CHEB / -7.4514000e-01 -5.5887000e-02 3.7299000e-02 /
CHEB / -3.9092000e-01 -1.0119000e-01 -1.1189000e-02 /

C2H4+OH(+m)=C2H5O-3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -24.8973064343348 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5680000e-01 3.3847000e+00 -5.0981000e-01 /
CHEB / 3.8820000e+00 1.1645000e+00 4.4249000e-01 /
CHEB / -8.6063000e-01 -2.5486000e-03 1.9762000e-02 /
CHEB / -6.2362000e-01 -1.1162000e-01 -2.9234000e-02 /
CHEB / -3.3766000e-01 -6.8275000e-02 -4.7709000e-02 /

C2H4+OH(+m)=CH3CHO+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -9.379202492569448
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 9.1866000e+00 -1.3137000e+00 -3.8307000e-01 /
CHEB / 2.5564000e+00 1.3720000e+00 3.1911000e-01 /
CHEB / -7.8559000e-02 1.3481000e-01 1.2535000e-01 /
CHEB / -2.0416000e-01 -1.1537000e-01 -1.1588000e-02 /
CHEB / -1.0265000e-01 -7.1677000e-02 -3.4474000e-02 /

C2H4+OH(+m)=CH3+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -13.208813463325189
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3688000e+00 -5.6886000e-01 -2.0139000e-01 /
CHEB / 5.7498000e+00 7.5927000e-01 2.4500000e-01 /
CHEB / 8.9630000e-02 -1.6636000e-01 -2.9771000e-02 /
CHEB / -2.1544000e-01 -3.1764000e-02 -3.1413000e-03 /
CHEB / -1.7105000e-01 9.5460000e-03 -9.6401000e-03 /

C2H4O+H(+m)=C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H/Nd_Cd/H2
H_rad       deltaHrxn(T=298K) = -28.766674644201927 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7721000e+00 1.6052000e+00 -3.6649000e-01 /
CHEB / -7.4770000e-01 7.1876000e-01 1.6445000e-01 /
CHEB / -1.1918000e+00 2.3350000e-01 8.8814000e-02 /
CHEB / -6.4514000e-01 6.5619000e-03 2.9515000e-02 /
CHEB / -3.2770000e-01 -5.2251000e-02 -4.8352000e-04 /

C2H4O+H(+m)=C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H/Nd
H_rad       deltaHrxn(T=298K) = -35.895793153016704 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0901000e+01 1.4105000e+00 -3.7344000e-01 /
CHEB / -1.6163000e+00 1.2070000e+00 -4.4845000e-03 /
CHEB / -1.3370000e+00 3.7326000e-01 1.0372000e-01 /
CHEB / -7.1384000e-01 2.9142000e-02 5.3043000e-02 /
CHEB / -3.5848000e-01 -5.9884000e-02 4.5639000e-03 /

C2H4O+H(+m)=C2H5O-3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -25.636832798233144 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7842000e+00 3.3367000e+00 -5.7895000e-01 /
CHEB / 2.7449000e+00 8.6523000e-01 3.5312000e-01 /
CHEB / -9.1068000e-01 1.8780000e-01 1.5757000e-01 /
CHEB / -5.8416000e-01 -4.9364000e-02 -1.2549000e-02 /
CHEB / -3.1498000e-01 -6.9563000e-02 -5.7024000e-02 /

C2H4O+H(+m)=C2H4+OH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -0.739526363898344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1233000e+01 -5.9136000e-01 -2.0453000e-01 /
CHEB / 1.5418000e+00 6.0070000e-01 1.7708000e-01 /
CHEB / -4.3134000e-02 7.9142000e-02 5.7172000e-02 /
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CHEB / -9.5022000e-02 -4.6029000e-02 -4.2752000e-03 /
CHEB / -5.6584000e-02 -3.5182000e-02 -1.5697000e-02 /

C2H4O+H(+m)=CH3CHO+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -10.11872885646779
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1686000e+01 -8.9255000e-01 -1.8968000e-01 /
CHEB / 1.0258000e+00 8.8111000e-01 1.1329000e-01 /
CHEB / -1.0827000e-01 1.5423000e-01 1.0637000e-01 /
CHEB / -1.1460000e-01 -6.6920000e-02 1.3608000e-02 /
CHEB / -4.7884000e-02 -6.4850000e-02 -2.4835000e-02 /

C2H4O+H(+m)=CH3+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -13.948339827223531
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0156000e+00 -6.8804000e-01 -2.8964000e-01 /
CHEB / 4.5992000e+00 7.6243000e-01 2.8801000e-01 /
CHEB / 2.0245000e-01 4.8674000e-02 6.2247000e-02 /
CHEB / -5.9065000e-02 -9.5946000e-02 -3.6329000e-02 /
CHEB / -9.9215000e-02 -4.4268000e-02 -2.8443000e-02 /

CH3CHO+H(+m)=C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -18.647945787734137
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8040000e+00 6.6128000e-01 -5.5442000e-01 /
CHEB / 3.6463000e+00 1.3592000e+00 2.6899000e-01 /
CHEB / -1.0662000e+00 2.9281000e-01 1.4829000e-01 /
CHEB / -6.9605000e-01 -6.5406000e-02 2.8310000e-02 /
CHEB / -3.6785000e-01 -1.0148000e-01 -1.5594000e-02 /

CH3CHO+H(+m)=C2H5O-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) OCO     H_rad      deltaHrxn(T=298K) = -25.777064296548915
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3389000e+00 5.7957000e-01 -7.8919000e-02 /
CHEB / 4.3954000e-02 8.4368000e-01 -5.1035000e-02 /
CHEB / -1.1242000e+00 3.7173000e-01 3.9946000e-02 /
CHEB / -6.7324000e-01 6.8275000e-02 4.3938000e-02 /
CHEB / -3.6122000e-01 -4.4865000e-02 1.3199000e-02 /

CH3CHO+H(+m)=C2H5O-3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) CO/H/Nd_O     H_rad      deltaHrxn(T=298K) = -
15.518103941765354 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1506000e+00 1.8900000e+00 -3.6537000e-01 /
CHEB / 2.1240000e+00 5.7873000e-01 1.9650000e-01 /
CHEB / -1.1533000e+00 2.4478000e-01 9.8299000e-02 /
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CHEB / -6.1504000e-01 3.0434000e-02 2.8717000e-02 /
CHEB / -3.0379000e-01 -3.6273000e-02 -2.8801000e-03 /

CH3CHO+H(+m)=CH3+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -3.8296109707557413
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9912000e+00 -4.5912000e-01 -1.9781000e-01 /
CHEB / 4.2622000e+00 4.6162000e-01 1.8241000e-01 /
CHEB / 6.1384000e-02 7.4055000e-02 4.5756000e-02 /
CHEB / -2.9546000e-02 -3.9766000e-02 -7.6494000e-03 /
CHEB / -4.6502000e-02 -3.0546000e-02 -1.4475000e-02 /

CH3+CH2O(+m)=C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -14.818334816978396
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.3785000e+00 2.7086000e+00 -6.6474000e-01 /
CHEB / 7.8710000e+00 1.3606000e+00 5.3973000e-01 /
CHEB / -9.5946000e-01 4.3271000e-02 6.9884000e-02 /
CHEB / -6.3739000e-01 -1.1441000e-01 8.2061000e-03 /
CHEB / -3.3386000e-01 -8.0034000e-02 -1.7254000e-02 /

CH3+CH2O(+m)=C2H5O-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1)      deltaHrxn(T=298K) = -21.947453325793173
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6051000e+00 2.7661000e+00 -8.4242000e-01 /
CHEB / 6.2259000e+00 1.3834000e+00 3.8499000e-01 /
CHEB / -1.1448000e+00 3.1192000e-01 2.2075000e-01 /
CHEB / -6.5657000e-01 -3.0431000e-02 4.7850000e-02 /
CHEB / -3.4655000e-01 -8.1411000e-02 -1.9116000e-02 /

CH3+CH2O(+m)=C2H5O-3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O-1) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) C_methyl     CO/H2_O           deltaHrxn(T=298K) = -
11.688492971009612 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4128000e+00 1.0610000e+00 -1.9639000e-01 /
CHEB / 2.0060000e+00 6.8819000e-01 1.1600000e-01 /
CHEB / -1.1727000e+00 2.5833000e-01 5.6991000e-02 /
CHEB / -6.2318000e-01 1.5729000e-02 1.3917000e-02 /
CHEB / -3.1564000e-01 -5.2988000e-02 -1.0039000e-02 /

C2H5+O(+m)=C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -94.85039801324879 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9341000e+00 1.3059000e+01 2.0747000e+00 /
CHEB / -2.0352000e+00 -1.9797000e+00 -1.5643000e-01 /
CHEB / -1.0257000e+00 -8.6530000e-01 -5.7220000e-01 /
CHEB / -5.4486000e-01 -4.9770000e-01 -1.6547000e-01 /
CHEB / -3.5869000e-01 -3.1949000e-01 1.0782000e-01 /
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C2H5+O(+m)=C2H5O-2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -101.97951652206356 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4162000e+00 1.4677000e+01 1.2702000e+00 /
CHEB / -2.9016000e+00 -2.6322000e+00 3.0700000e-01 /
CHEB / -9.7109000e-01 -1.2473000e+00 -4.6153000e-01 /
CHEB / -5.4207000e-01 -5.2081000e-01 -8.5564000e-02 /
CHEB / -3.9673000e-01 -2.3609000e-01 1.4622000e-01 /

C2H5+O(+m)=C2H5O-3(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1) High-P Limit: Oa_R_Recombination estimate: (Average:)
C_rad/H2/Cs     Oa      deltaHrxn(T=298K) = -91.72055616728001 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1170000e+01 1.1659000e+01 3.0019000e+00 /
CHEB / -1.0937000e+00 -2.7380000e-01 -1.1961000e+00 /
CHEB / -7.7384000e-01 -5.6020000e-01 -8.5317000e-01 /
CHEB / -6.3880000e-01 -6.1605000e-01 -1.4084000e-01 /
CHEB / -4.5665000e-01 -4.5598000e-01 1.7225000e-01 /

C2H5+O(+m)=C2H4+OH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -66.8232497329452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1932000e+01 -9.7726000e-04 -6.8234000e-04 /
CHEB / 6.6577000e-01 8.4815000e-04 5.9262000e-04 /
CHEB / -1.1502000e-01 3.8212000e-04 2.6605000e-04 /
CHEB / -1.2695000e-01 -9.9216000e-05 -6.8997000e-05 /
CHEB / -6.5312000e-02 -1.5624000e-04 -1.0901000e-04 /

C2H5+O(+m)=C2H4O+H(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -66.08372336904685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1505000e+01 -1.7751000e-03 -1.2746000e-03 /
CHEB / 1.3580000e+00 1.8643000e-03 1.3608000e-03 /
CHEB / 1.6146000e-01 6.0914000e-05 8.3125000e-06 /
CHEB / -2.9443000e-02 4.8428000e-05 4.6421000e-05 /
CHEB / -3.0263000e-02 -1.7944000e-04 -1.2757000e-04 /

C2H5+O(+m)=CH3CHO+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -76.20245222551466 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1352000e+01 1.5219000e-04 1.0859000e-04 /
CHEB / 4.2827000e-01 -2.2653000e-05 -1.7443000e-05 /
CHEB / 4.9466000e-02 -5.1734000e-05 -3.8541000e-05 /
CHEB / -1.8405000e-02 -5.2736000e-05 -3.4970000e-05 /
CHEB / -2.4231000e-02 -4.2288000e-05 -2.9525000e-05 /

C2H5+O(+m)=CH3+CH2O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C2H5O-1)      deltaHrxn(T=298K) = -80.03206319627039 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2730000e+01 1.2301000e-04 8.5759000e-05 /
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CHEB / -6.4895000e-01 8.1610000e-05 5.6909000e-05 /
CHEB / -3.7756000e-01 -1.0543000e-04 -7.3513000e-05 /
CHEB / -1.7858000e-01 -1.2290000e-04 -8.5721000e-05 /
CHEB / -6.8373000e-02 -4.1934000e-05 -2.9253000e-05 /

!PDepNetwork C3H6
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!Here are the path reactions and their high-P limit kinetics:
!     pC3H5+H=C3H6            1.000e+14    0.00        0.00
!     C2H3+CH3=C3H6           2.000e+13    0.00        0.00
!     sC3H5+H=C3H6            1.000e+14    0.00        0.00
!     aC3H5+H=C3H6            1.000e+14    0.00        0.00

pC3H5+H(+m)=C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -111.35805120498212 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2369000e+01 1.6764000e+00 -5.1011000e-01 /
CHEB / -2.3183000e+00 1.6640000e+00 -1.6889000e-01 /
CHEB / -1.4239000e+00 7.5210000e-01 2.9111000e-02 /
CHEB / -7.7165000e-01 2.5325000e-01 5.4139000e-02 /
CHEB / -4.0237000e-01 5.7502000e-02 2.8315000e-02 /

C2H3+CH3(+m)=C3H6(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -101.19914872304854 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2413000e+01 7.6444000e-01 -1.6180000e-01 /
CHEB / -1.6173000e+00 1.1982000e+00 -1.8282000e-01 /
CHEB / -1.1440000e+00 6.8306000e-01 -3.1068000e-02 /
CHEB / -6.6639000e-01 2.8595000e-01 3.3999000e-02 /
CHEB / -3.7385000e-01 8.0900000e-02 3.2311000e-02 /

pC3H5+H(+m)=C2H3+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6)   deltaHrxn(T=298K) = -10.158902481933573 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.3188000e+01 -9.2981000e-01 -1.7757000e-01 /
CHEB / 7.4591000e-01 9.0702000e-01 1.0184000e-01 /
CHEB / 1.5038000e-01 1.7720000e-01 9.9591000e-02 /
CHEB / -2.6993000e-02 -7.8003000e-02 1.7535000e-02 /
CHEB / -2.4692000e-02 -7.0596000e-02 -2.3471000e-02 /

sC3H5+H(+m)=C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -107.80841670844771 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2692000e+01 1.2261000e+00 -3.3553000e-01 /
CHEB / -2.0510000e+00 1.5379000e+00 -2.1711000e-01 /
CHEB / -1.3310000e+00 7.4712000e-01 -2.7259000e-03 /
CHEB / -7.4466000e-01 2.6945000e-01 4.7130000e-02 /
CHEB / -3.9768000e-01 6.5785000e-02 2.9773000e-02 /

pC3H5+H(+m)=sC3H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6)   deltaHrxn(T=298K) = -3.5496344965344093 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0480000e+01 -8.9241000e-01 -1.7328000e-01 /
CHEB / 1.7751000e+00 9.0996000e-01 1.0618000e-01 /
CHEB / 4.0905000e-01 1.3208000e-01 9.8247000e-02 /
CHEB / 4.1303000e-02 -9.0064000e-02 8.0853000e-03 /
CHEB / 5.0891000e-03 -6.1812000e-02 -2.6869000e-02 /

sC3H5+H(+m)=C2H3+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6)   deltaHrxn(T=298K) = -6.609267985399164 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2844000e+01 -1.0564000e+00 -1.3649000e-01 /
CHEB / 1.0726000e+00 1.0060000e+00 4.0831000e-02 /
CHEB / 1.8255000e-01 2.2099000e-01 1.0605000e-01 /
CHEB / -5.1127000e-02 -7.6931000e-02 3.3553000e-02 /
CHEB / -3.8153000e-02 -8.0831000e-02 -1.9904000e-02 /

aC3H5+H(+m)=C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -87.89050925332106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3611000e+01 3.2295000e-01 -3.6171000e-02 /
CHEB / -9.2302000e-01 5.8579000e-01 -5.7709000e-02 /
CHEB / -7.1811000e-01 4.3522000e-01 -2.4507000e-02 /
CHEB / -5.0165000e-01 2.5970000e-01 6.1615000e-03 /
CHEB / -3.2436000e-01 1.1728000e-01 2.0422000e-02 /

pC3H5+H(+m)=aC3H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6)   deltaHrxn(T=298K) = -23.46754195166107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2824000e+01 -9.5616000e-01 -1.9609000e-01 /
CHEB / 6.5361000e-01 8.7379000e-01 1.0322000e-01 /
CHEB / 3.6833000e-02 2.2412000e-01 1.0542000e-01 /
CHEB / -5.2714000e-02 -4.5279000e-02 3.0305000e-02 /
CHEB / -3.4561000e-02 -7.1681000e-02 -1.6461000e-02 /
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aC3H5+H(+m)=C2H3+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6)   deltaHrxn(T=298K) = 13.308639469727488 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8999000e+00 -1.2860000e+00 -8.2163000e-02 /
CHEB / 5.4354000e+00 1.0250000e+00 -3.5963000e-02 /
CHEB / -5.9265000e-02 4.0085000e-01 7.3382000e-02 /
CHEB / -1.6800000e-01 1.5409000e-02 6.6663000e-02 /
CHEB / -1.0021000e-01 -8.7668000e-02 1.3612000e-02 /

sC3H5+H(+m)=aC3H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H6)   deltaHrxn(T=298K) = -19.917907455126645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2672000e+01 -1.1158000e+00 -1.4209000e-01 /
CHEB / 8.2660000e-01 9.7962000e-01 2.9045000e-02 /
CHEB / 5.7520000e-02 2.8874000e-01 1.0337000e-01 /
CHEB / -7.0054000e-02 -3.2845000e-02 4.9573000e-02 /
CHEB / -4.9634000e-02 -8.1448000e-02 -7.0817000e-03 /

!PDepNetwork C2H5OH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H5O-3           -2.66 66.84 15.8  18.82 21.65 24.13 28.15 31.21
      36.01
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!Here are the path reactions and their high-P limit kinetics:
!     CH3+CH2OH=C2H5OH        1.000e+13    0.00        0.00
!     C2H5O-1+H=C2H5OH        1.0000000e+14      0.00000
0.0000000e+00
!     C2H5+OH=C2H5OH          7.7000000e+13      0.00000
0.0000000e+00
!     C2H5O-2+H=C2H5OH        5.0000000e+13      0.00000
0.0000000e+00
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!     C2H5O-3+H=C2H5OH        1.4157154e+13      -0.15000
2.9166667e+02
!     C2H5OH=C2H4+H2O         3.200e+04    2.53        62940.00

CH3+CH2OH(+m)=C2H5OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) High-P Limit: R_Recombination Primary Kinetic
Library: Mike     deltaHrxn(T=298K) = -87.6403978741543 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2085000e+01 9.0338000e-01 -2.0749000e-01 /
CHEB / -2.0061000e+00 1.5316000e+00 -3.1323000e-01 /
CHEB / -1.4138000e+00 9.9013000e-01 -1.4809000e-01 /
CHEB / -8.6211000e-01 5.0635000e-01 -3.5309000e-02 /
CHEB / -4.9488000e-01 2.0551000e-01 1.0634000e-02 /

CH3+CH2OH(+m)=C2H4+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -76.31192011793325 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0615000e+01 -1.3496000e+00 -6.6447000e-02 /
CHEB / 1.3378000e+00 9.9323000e-01 -4.7155000e-02 /
CHEB / 4.0155000e-02 4.5045000e-01 4.9624000e-02 /
CHEB / -1.1935000e-01 7.0553000e-02 6.2368000e-02 /
CHEB / -8.2050000e-02 -6.7321000e-02 2.7329000e-02 /

C2H5O-1+H(+m)=C2H5OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -102.53873778493681
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1394000e+01 2.8197000e+00 -8.2185000e-01 /
CHEB / -2.9089000e+00 1.9247000e+00 -1.0079000e-01 /
CHEB / -1.8164000e+00 1.0118000e+00 -4.0417000e-02 /
CHEB / -1.0152000e+00 4.6733000e-01 -8.2154000e-03 /
CHEB / -5.4253000e-01 1.9132000e-01 1.6646000e-02 /

C2H5O-1+H(+m)=CH3+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -14.898339910782523 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3641000e+01 -6.1460000e-01 -2.2179000e-01 /
CHEB / 3.3886000e-01 6.2879000e-01 1.9441000e-01 /
CHEB / 3.2655000e-02 8.9594000e-02 6.6174000e-02 /
CHEB / -1.4688000e-02 -6.2037000e-02 -1.1360000e-02 /
CHEB / -6.1421000e-03 -4.3944000e-02 -2.2233000e-02 /

C2H5O-1+H(+m)=C2H5+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -8.18877867330444 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2662000e+01 -6.0701000e-01 -2.0878000e-01 /
CHEB / 7.2897000e-01 6.4672000e-01 1.8984000e-01 /
CHEB / 1.6873000e-01 6.3098000e-02 5.8641000e-02 /
CHEB / 2.2319000e-02 -7.1819000e-02 -1.6344000e-02 /
CHEB / 5.3690000e-03 -3.8842000e-02 -2.1670000e-02 /
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C2H5O-1+H(+m)=C2H5O-2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -7.129118508814777 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0895000e+01 -6.0538000e-01 -2.0784000e-01 /
CHEB / 1.3190000e+00 6.4720000e-01 1.8963000e-01 /
CHEB / 3.2434000e-01 6.0554000e-02 5.7952000e-02 /
CHEB / 7.5513000e-02 -7.2345000e-02 -1.6752000e-02 /
CHEB / 2.6118000e-02 -3.8242000e-02 -2.1573000e-02 /

C2H5O-1+H(+m)=C2H4+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -91.2102600287158 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1556000e+01 -5.7124000e-01 -2.6029000e-01 /
CHEB / 9.3770000e-01 5.5700000e-01 2.1469000e-01 /
CHEB / 2.5396000e-02 1.1070000e-01 8.3619000e-02 /
CHEB / -3.7753000e-02 -3.9973000e-02 -2.8678000e-04 /
CHEB / -1.8524000e-02 -4.4230000e-02 -2.1854000e-02 /

C2H5+OH(+m)=C2H5OH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (C2H5OH) High-P Limit: R_Recombination exact:  C_rad/H2/Cs
O_pri_rad         deltaHrxn(T=298K) = -94.34995911163239 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2471000e+01 1.4545000e+00 -4.0117000e-01 /
CHEB / -2.5412000e+00 1.9133000e+00 -3.3318000e-01 /
CHEB / -1.6549000e+00 1.0822000e+00 -1.2371000e-01 /
CHEB / -9.6995000e-01 5.1152000e-01 -2.6985000e-02 /
CHEB / -5.3647000e-01 2.0486000e-01 9.7179000e-03 /

C2H5+OH(+m)=CH3+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -6.709561237478082 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3134000e+01 -9.9635000e-01 -1.4850000e-01 /
CHEB / 7.4985000e-01 9.6427000e-01 6.7351000e-02 /
CHEB / 7.2582000e-02 1.9182000e-01 9.8128000e-02 /
CHEB / -6.3625000e-02 -7.6215000e-02 2.1859000e-02 /
CHEB / -3.7796000e-02 -7.3649000e-02 -1.9965000e-02 /

C2H5+OH(+m)=C2H4+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -83.02148135541134 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1612000e+01 -1.0822000e+00 -1.6106000e-01 /
CHEB / 9.9470000e-01 9.3337000e-01 4.6886000e-02 /
CHEB / -3.4113000e-04 2.8494000e-01 1.0074000e-01 /
CHEB / -9.0784000e-02 -1.5018000e-02 4.8407000e-02 /
CHEB / -5.6357000e-02 -7.1583000e-02 -1.5933000e-03 /

C2H5O-2+H(+m)=C2H5OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/CsO     H_rad          deltaHrxn(T=298K) = -
95.40961927612204 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.2159000e+01 1.5161000e+00 -4.2425000e-01 /
CHEB / -2.5070000e+00 1.9295000e+00 -3.2541000e-01 /
CHEB / -1.6621000e+00 1.0830000e+00 -1.1939000e-01 /
CHEB / -9.7141000e-01 5.1015000e-01 -2.5972000e-02 /
CHEB / -5.3266000e-01 2.0437000e-01 9.9541000e-03 /

C2H5O-2+H(+m)=CH3+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -7.769221401967746 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2911000e+01 -9.7521000e-01 -1.5542000e-01 /
CHEB / 7.7594000e-01 9.4796000e-01 7.7171000e-02 /
CHEB / 7.6390000e-02 1.8412000e-01 9.7429000e-02 /
CHEB / -5.6925000e-02 -7.6278000e-02 1.9426000e-02 /
CHEB / -3.0937000e-02 -7.1827000e-02 -2.0613000e-02 /

C2H5O-2+H(+m)=C2H5+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -1.0596601644896637 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1602000e+01 -8.9033000e-01 -1.6261000e-01 /
CHEB / 1.4906000e+00 9.2075000e-01 9.8187000e-02 /
CHEB / 1.9747000e-01 1.1335000e-01 9.6377000e-02 /
CHEB / -2.9972000e-02 -8.7890000e-02 3.6487000e-03 /
CHEB / -1.5681000e-02 -5.8421000e-02 -2.5127000e-02 /

C2H5O-2+H(+m)=C2H4+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -84.08114151990101 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1349000e+01 -1.0521000e+00 -1.7196000e-01 /
CHEB / 1.0487000e+00 9.1597000e-01 6.0244000e-02 /
CHEB / 6.8162000e-03 2.7148000e-01 1.0293000e-01 /
CHEB / -8.4242000e-02 -1.8685000e-02 4.5516000e-02 /
CHEB / -4.9010000e-02 -7.0233000e-02 -3.8840000e-03 /

C2H5O-3+H(+m)=C2H5OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
105.66857963090561 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2461000e+00 3.5611000e+00 -9.3522000e-01 /
CHEB / -2.9674000e+00 1.8237000e+00 8.9573000e-05 /
CHEB / -1.8909000e+00 9.5026000e-01 -1.4792000e-02 /
CHEB / -1.0534000e+00 4.4124000e-01 -2.6404000e-03 /
CHEB / -5.5731000e-01 1.8337000e-01 2.0439000e-02 /

C2H5O-3+H(+m)=CH3+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -18.02818175675131 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2282000e+01 -4.6217000e-01 -2.1101000e-01 /
CHEB / 2.9205000e-01 4.8409000e-01 2.0201000e-01 /
CHEB / -8.5582000e-03 5.7443000e-02 4.6859000e-02 /
CHEB / -2.8484000e-02 -5.1736000e-02 -1.7804000e-02 /
CHEB / -1.1327000e-02 -3.2145000e-02 -1.8917000e-02 /
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C2H5O-3+H(+m)=C2H5O-1+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -3.129841845968784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9411000e+00 -4.5292000e-01 -1.8671000e-01 /
CHEB / 1.8902000e+00 5.1710000e-01 1.9285000e-01 /
CHEB / 4.5831000e-01 7.5836000e-03 2.9554000e-02 /
CHEB / 1.0446000e-01 -6.1922000e-02 -2.4136000e-02 /
CHEB / 3.3000000e-02 -2.0314000e-02 -1.5044000e-02 /

C2H5O-3+H(+m)=C2H5+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -11.318620519273225 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1402000e+01 -4.6823000e-01 -2.0203000e-01 /
CHEB / 6.0303000e-01 5.0566000e-01 1.9877000e-01 /
CHEB / 1.1808000e-01 4.2688000e-02 4.0895000e-02 /
CHEB / 1.0274000e-02 -5.8692000e-02 -2.0721000e-02 /
CHEB / 1.1848000e-04 -2.9393000e-02 -1.7940000e-02 /

C2H5O-3+H(+m)=C2H5O-2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -10.25896035478356 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6435000e+00 -4.6826000e-01 -2.0127000e-01 /
CHEB / 1.1845000e+00 5.0711000e-01 1.9850000e-01 /
CHEB / 2.7348000e-01 4.1153000e-02 4.0362000e-02 /
CHEB / 6.3792000e-02 -5.9170000e-02 -2.0950000e-02 /
CHEB / 2.0840000e-02 -2.9044000e-02 -1.7831000e-02 /

C2H5O-3+H(+m)=C2H4+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C2H5OH) deltaHrxn(T=298K) = -94.34010187468456 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0008000e+01 -3.9575000e-01 -2.3355000e-01 /
CHEB / 9.9114000e-01 4.0795000e-01 2.1670000e-01 /
CHEB / 1.2461000e-02 6.2355000e-02 5.7942000e-02 /
CHEB / -4.5204000e-02 -3.9365000e-02 -1.2793000e-02 /
CHEB / -2.0284000e-02 -3.2521000e-02 -2.0799000e-02 /

C2H4+H2O(+m)=C2H5OH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#4 (C2H5OH) deltaHrxn(T=298K) = -11.328477756221034 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1826000e+01 2.7533000e-01 -3.6564000e-02 /
CHEB / 1.8295000e+01 5.1346000e-01 -6.3680000e-02 /
CHEB / -1.6724000e-01 4.1441000e-01 -3.9616000e-02 /
CHEB / -3.0442000e-01 2.8488000e-01 -1.1165000e-02 /
CHEB / -2.7073000e-01 1.6057000e-01 1.1316000e-02 /

!PDepNetwork CH3CHO && C2H4O
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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!     CH3CHO            -39.72      63.07 13.26 15.78 18.29 20.58 24.16
      26.91 30.96 Primary Thermo Library: GRI-Mech3.0 (Species ID:
s00002656)
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 Estimated by Group Additivity
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 Estimated by Group Additivity
!     H                 52.1  27.41 4.97  4.97  4.97  4.97  4.97  4.97
      4.97  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009800)
!     C2H3              71.63 55.89 10.24 12.03 13.71 15.17 17.34 19.07
      21.81 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002447)
!     OH                9.4   43.91 7.14  7.07  7.05  7.06  7.15  7.34
      7.87  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00010102)
!     C2H3O-2           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 Estimated by Group Additivity
!     CH2CHO            6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34
      26.35 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002559)
!     CH3         35.1  46.36 9.2   9.98  10.75 11.5  12.86 14.08 16.29
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009089)
!     HCO         10.04 53.61 8.27  8.72  9.24  9.78  10.74 11.49 12.59
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009325)
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      Estimated by Group Additivity
!     CH4               -17.83      44.53 8.55  9.69  11.11 12.6  15.29
      17.59 21.61 Primary Thermo Library: GRI-Mech3.0 (Species ID:
s00009193)
!     CO          -26.42      47.23 6.96  7.02  7.12  7.27  7.62  7.93
      8.41  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009358)
!Here are the path reactions and their high-P limit kinetics:
!     C2H4O=CH3CHO                  8.590e+11    0.32        55900.00
!     C2H3O-1+H=C2H4O         5.360e+14    0.00        980.00
!     C2H3+OH=C2H4O           1.000e+13    0.00        0.00
!     C2H3O-2+H=C2H4O         1.000e+13    0.00        0.00
!     CH2CHO+H=C2H4O          1.000e+13    0.00        0.00
!     CH3+HCO=CH3CHO          1.810e+13    0.00        0.00
!     CH2CHO+H=CH3CHO         5.000e+13    0.00        0.00
!     CH3CO+H=CH3CHO          1.000e+13    0.00        0.00
!     CH4+CO=CH3CHO           1.640e+04    2.86        86900.00

C2H4O(+m)=CH3CHO(+m)                              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) High-P Limit:
ReactionLibrary: Tautomerization    deltaHrxn(T=298K) = -
10.106913211832161 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.0863000e+01 2.9891000e-01 -5.6431000e-02 4.1724000e-03 /
CHEB / 1.6830000e+01 5.0599000e-01 -7.9601000e-02 2.8636000e-04 /
CHEB / -3.7824000e-01 3.1597000e-01 -2.2136000e-02 -8.6711000e-03 /
CHEB / -2.3870000e-01 1.4662000e-01 1.2800000e-02 -8.0347000e-03 /

C2H3O-1+H(+m)=CH3CHO(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -
121.29150016156129 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.5780000e+00 8.4259000e+00 -1.3146000e+00 -4.7454000e-01 /
CHEB / -1.9241000e+00 5.3003000e-01 1.2409000e+00 -4.4033000e-02 /
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CHEB / -6.7566000e-01 -4.0974000e-01 4.4371000e-01 8.9082000e-02 /
CHEB / -2.6329000e-01 -2.0681000e-01 9.5202000e-02 4.5187000e-02 /

C2H3O-1+H(+m)=C2H4O(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) High-P Limit:
R_Recombination exact:  [ Cd_pri_rad , H_rad ]  deltaHrxn(T=298K) = -
111.18458694972914 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.9911000e+00 9.1818000e+00 -1.1737000e+00 -5.1404000e-01 /
CHEB / -2.3221000e+00 3.2075000e-01 1.2773000e+00 -1.0027000e-02 /
CHEB / -7.5798000e-01 -4.7710000e-01 4.4091000e-01 1.0430000e-01 /
CHEB / -2.8657000e-01 -2.2882000e-01 8.9270000e-02 4.9540000e-02 /

C2H3+OH(+m)=CH3CHO(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -120.73765144278903
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.3597000e+00 8.2808000e+00 -1.3184000e+00 -4.6480000e-01 /
CHEB / -2.1686000e+00 5.6043000e-01 1.2258000e+00 -5.2185000e-02 /
CHEB / -6.7745000e-01 -3.9060000e-01 4.4154000e-01 8.6483000e-02 /
CHEB / -2.6518000e-01 -2.0177000e-01 9.5993000e-02 4.4636000e-02 /

C2H3+OH(+m)=C2H4O(+m)                     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO) High-P Limit: R_Recombination estimate:
(Average:) [ Cd_pri_rad , O_pri_rad ]     deltaHrxn(T=298K) = -
110.63073823095688 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.7727000e+00 9.0367000e+00 -1.1775000e+00 -5.0429000e-01 /
CHEB / -2.5667000e+00 3.5116000e-01 1.2622000e+00 -1.8179000e-02 /
CHEB / -7.5978000e-01 -4.5797000e-01 4.3874000e-01 1.0170000e-01 /
CHEB / -2.8847000e-01 -2.2377000e-01 9.0061000e-02 4.8988000e-02 /

C2H3O-1+H(+m)=C2H3+OH(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -0.5538487187722616
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1612000e+01 -2.6917000e-01 -1.4324000e-01 -4.4473000e-02 /
CHEB / 1.6841000e+00 3.0774000e-01 1.5273000e-01 3.6852000e-02 /
CHEB / 2.9227000e-01 -1.2635000e-02 7.5265000e-03 1.5395000e-02 /
CHEB / 3.6011000e-02 -2.3450000e-02 -1.3610000e-02 -4.4483000e-03 /

C2H3O-2+H(+m)=CH3CHO(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -
121.29150016156129 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.6456000e+00 8.1357000e+00 -1.3216000e+00 -4.5494000e-01 /
CHEB / -2.2468000e+00 5.9015000e-01 1.2105000e+00 -6.0316000e-02 /
CHEB / -6.7880000e-01 -3.7174000e-01 4.3940000e-01 8.3760000e-02 /
CHEB / -2.6442000e-01 -1.9691000e-01 9.6933000e-02 4.3938000e-02 /

C2H3O-2+H(+m)=C2H4O(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) High-P Limit:
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R_Recombination estimate: (Average:) [ Cd_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -111.18458694972914 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.0586000e+00 8.8915000e+00 -1.1807000e+00 -4.9444000e-01 /
CHEB / -2.6448000e+00 3.8087000e-01 1.2469000e+00 -2.6309000e-02 /
CHEB / -7.6113000e-01 -4.3910000e-01 4.3660000e-01 9.8976000e-02 /
CHEB / -2.8771000e-01 -2.1892000e-01 9.1001000e-02 4.8289000e-02 /

C2H3O-1+H(+m)=C2H3O-2+H(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7960000e+00 -2.6971000e-01 -1.4394000e-01 -4.4798000e-02 /
CHEB / 2.1114000e+00 3.0698000e-01 1.5298000e-01 3.7098000e-02 /
CHEB / 3.9912000e-01 -1.0599000e-02 8.1318000e-03 1.5385000e-02 /
CHEB / 6.9782000e-02 -2.4130000e-02 -1.3676000e-02 -4.2816000e-03 /

C2H3O-2+H(+m)=C2H3+OH(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -0.5538487187722616
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0162000e+01 -2.7487000e-01 -1.4546000e-01 -4.4479000e-02 /
CHEB / 1.5070000e+00 3.1338000e-01 1.5436000e-01 3.6235000e-02 /
CHEB / 2.9210000e-01 -1.1935000e-02 8.4088000e-03 1.6010000e-02 /
CHEB / 3.5623000e-02 -2.3868000e-02 -1.3700000e-02 -4.2919000e-03 /

CH2CHO+H(+m)=CH3CHO(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/CO , H_rad ]
      deltaHrxn(T=298K) = -97.80091539167051 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0585000e+01 3.2188000e+00 -6.0697000e-01 1.5031000e-02 /
CHEB / -1.5187000e+00 6.3251000e-01 1.1196000e-01 -1.4633000e-01 /
CHEB / -6.5376000e-01 1.2169000e-01 1.1462000e-01 -3.3273000e-02 /
CHEB / -2.6637000e-01 3.6753000e-02 3.3582000e-02 2.3692000e-03 /

CH2CHO+H(+m)=C2H4O(+m)                           1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (CH3CHO) High-P Limit:
R_Recombination estimate: (Average:) [ O_rad/OneDe , H_rad ]
      deltaHrxn(T=298K) = -87.69400217983836 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0508000e+01 3.1871000e+00 -8.3576000e-01 -4.8226000e-02 /
CHEB / -1.5668000e+00 9.7158000e-01 3.6543000e-01 -1.6265000e-01 /
CHEB / -6.6076000e-01 1.8367000e-01 1.9195000e-01 1.4082000e-02 /
CHEB / -2.8720000e-01 2.3828000e-02 4.6058000e-02 3.0653000e-02 /

C2H3O-1+H(+m)=CH2CHO+H(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -23.490584769890773
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3289000e+01 -2.2646000e-01 -1.3350000e-01 -5.1910000e-02 /
CHEB / 5.3350000e-01 2.4340000e-01 1.3579000e-01 4.4654000e-02 /
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CHEB / 7.7525000e-02 6.0788000e-03 1.2667000e-02 1.4364000e-02 /
CHEB / 1.9948000e-02 -1.7985000e-02 -1.0291000e-02 -3.4412000e-03 /

C2H3+OH(+m)=CH2CHO+H(+m)                  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -22.936736051118515
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1888000e+01 -2.3361000e-01 -1.3663000e-01 -5.2084000e-02 /
CHEB / 2.8862000e-01 2.5034000e-01 1.3826000e-01 4.4079000e-02 /
CHEB / 8.2679000e-02 7.0369000e-03 1.3638000e-02 1.5077000e-02 /
CHEB / 1.9893000e-02 -1.8430000e-02 -1.0353000e-02 -3.2331000e-03 /

C2H3O-2+H(+m)=CH2CHO+H(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -23.490584769890773
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1991000e+01 -2.4093000e-01 -1.3975000e-01 -5.2193000e-02 /
CHEB / 2.1012000e-01 2.5745000e-01 1.4070000e-01 4.3421000e-02 /
CHEB / 8.8178000e-02 8.0058000e-03 1.4631000e-02 1.5791000e-02 /
CHEB / 2.2349000e-02 -1.8879000e-02 -1.0405000e-02 -3.0079000e-03 /

CH3+HCO(+m)=CH3CHO(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO) High-P Limit: R_Recombination exact:  [
C_methyl , CO_pri_rad ] deltaHrxn(T=298K) = -84.84951408998302 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2525000e+01 7.3766000e-01 -1.3304000e-01 -2.3559000e-04 /
CHEB / -1.0043000e+00 5.5158000e-01 2.2085000e-02 -2.1536000e-03 /
CHEB / -5.5200000e-01 2.2380000e-01 2.3373000e-02 2.4894000e-03 /
CHEB / -2.4401000e-01 6.1816000e-02 1.0448000e-02 2.0945000e-03 /

CH3+HCO(+m)=C2H4O(+m)                     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -74.74260087815087
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1661000e+01 -2.3023000e-01 -3.9016000e-01 3.9044000e-02 /
CHEB / -6.1259000e-01 1.2777000e+00 9.1814000e-02 -7.9733000e-02 /
CHEB / -4.6781000e-01 4.1269000e-01 1.0398000e-01 -5.1152000e-03 /
CHEB / -2.4761000e-01 8.4266000e-02 4.0911000e-02 1.1533000e-02 /

C2H3O-1+H(+m)=CH3+HCO(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -36.44198607157827
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.4240000e+01 -1.3931000e-01 -1.0121000e-01 -5.7234000e-02 /
CHEB / 2.6899000e-01 1.6640000e-01 1.1550000e-01 5.9633000e-02 /
CHEB / -6.8618000e-02 -7.3470000e-03 2.0130000e-03 9.0273000e-03 /
CHEB / -2.6804000e-02 -1.5324000e-02 -1.1680000e-02 -7.2572000e-03 /

C2H3+OH(+m)=CH3+HCO(+m)             1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -35.88813735280601 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
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CHEB / 1.2863000e+01 -1.4589000e-01 -1.0496000e-01 -5.8318000e-02 /
CHEB / 1.3537000e-02 1.7302000e-01 1.1874000e-01 5.9860000e-02 /
CHEB / -6.7054000e-02 -6.5432000e-03 3.0427000e-03 1.0081000e-02 /
CHEB / -2.7646000e-02 -1.5769000e-02 -1.1799000e-02 -7.1072000e-03 /

C2H3O-2+H(+m)=CH3+HCO(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -36.44198607157827
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2991000e+01 -1.5266000e-01 -1.0878000e-01 -5.9358000e-02 /
CHEB / -7.5757000e-02 1.7978000e-01 1.2200000e-01 6.0002000e-02 /
CHEB / -6.5252000e-02 -5.6755000e-03 4.1101000e-03 1.1148000e-02 /
CHEB / -2.5990000e-02 -1.6213000e-02 -1.1896000e-02 -6.9242000e-03 /

CH2CHO+H(+m)=CH3+HCO(+m)            1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -12.951401301687493 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3754000e+01 -1.8486000e-01 -1.0489000e-01 -4.0739000e-02 /
CHEB / 3.7153000e-02 1.7689000e-01 9.6520000e-02 3.6473000e-02 /
CHEB / 1.4966000e-03 2.4790000e-02 1.6356000e-02 5.6098000e-03 /
CHEB / 6.5310000e-03 -1.0004000e-02 -4.6161000e-03 -1.3997000e-03 /

CH3CO+H(+m)=CH3CHO(+m)                   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO) High-P Limit: R_Recombination estimate:
(Average:) [ CO_rad/NonDe , H_rad ] deltaHrxn(T=298K) = -
89.52481149933112 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1567000e+01 1.5182000e+00 -3.6613000e-01 3.5934000e-02 /
CHEB / -1.1536000e+00 5.4934000e-01 7.3511000e-02 -3.3599000e-03 /
CHEB / -6.0192000e-01 1.9108000e-01 3.6742000e-02 -3.3079000e-03 /
CHEB / -2.6308000e-01 4.7321000e-02 9.2302000e-03 4.1130000e-04 /

CH3CO+H(+m)=C2H4O(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -79.41789828749897
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0871000e+01 7.1313000e-01 -6.6088000e-01 5.4471000e-02 /
CHEB / -8.6883000e-01 1.2024000e+00 1.9691000e-01 -7.9632000e-02 /
CHEB / -5.3733000e-01 3.5308000e-01 1.2267000e-01 -4.9934000e-04 /
CHEB / -2.6558000e-01 6.9529000e-02 3.8499000e-02 1.1577000e-02 /

C2H3O-1+H(+m)=CH3CO+H(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -31.766688662230166
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1558000e+01 -1.5998000e-01 -1.0947000e-01 -5.6426000e-02 /
CHEB / 6.9006000e-01 1.8349000e-01 1.2020000e-01 5.6095000e-02 /
CHEB / 3.5546000e-02 -3.5852000e-03 4.8295000e-03 1.0453000e-02 /
CHEB / 4.2643000e-03 -1.5486000e-02 -1.1033000e-02 -6.1480000e-03 /

C2H3+OH(+m)=CH3CO+H(+m)             1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -31.212839943457908 kcal/mol
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```
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0178000e+01 -1.6687000e-01 -1.1318000e-01 -5.7303000e-02 /
CHEB / 4.3597000e-01 1.9026000e-01 1.2331000e-01 5.6121000e-02 /
CHEB / 3.7641000e-02 -2.6854000e-03 5.8655000e-03 1.1419000e-02 /
CHEB / 3.5688000e-03 -1.5907000e-02 -1.1123000e-02 -5.9742000e-03 /

C2H3O-2+H(+m)=CH3CO+H(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -31.766688662230166
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0302000e+01 -1.7395000e-01 -1.1694000e-01 -5.8135000e-02 /
CHEB / 3.4809000e-01 1.9717000e-01 1.2642000e-01 5.6067000e-02 /
CHEB / 3.9987000e-02 -1.7254000e-03 6.9360000e-03 1.2392000e-02 /
CHEB / 5.3759000e-03 -1.6327000e-02 -1.1194000e-02 -5.7722000e-03 /

CH2CHO+H(+m)=CH3CO+H(+m)                  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -8.276103892339393
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0795000e+01 -1.9545000e-01 -1.0407000e-01 -3.7635000e-02 /
CHEB / 5.9152000e-01 1.9162000e-01 9.8373000e-02 3.4808000e-02 /
CHEB / 1.5039000e-01 2.1793000e-02 1.3670000e-02 4.1604000e-03 /
CHEB / 4.8905000e-02 -1.2144000e-02 -5.3578000e-03 -1.6587000e-03 /

CH3CO+H(+m)=CH3+HCO(+m)             1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -4.675297409348101 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2656000e+01 -5.6408000e-01 -1.9259000e-01 -1.2293000e-02 /
CHEB / 3.5884000e-01 5.5577000e-01 1.6611000e-01 -6.4848000e-03 /
CHEB / 2.6148000e-02 6.4750000e-02 4.0641000e-02 1.5443000e-02 /
CHEB / -1.5439000e-02 -3.8327000e-02 -6.2968000e-03 4.5617000e-03 /

CH3CHO(+m)=CH4+CO(+m)                     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -4.526609940821448
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.1310000e+01 5.0217000e-01 -6.1544000e-02 -1.6258000e-02 /
CHEB / 2.5393000e+01 4.8816000e-01 1.3330000e-02 -2.9072000e-03 /
CHEB / -3.7527000e-01 2.2618000e-01 1.5954000e-02 5.9816000e-03 /
CHEB / -2.2198000e-01 6.9903000e-02 1.1059000e-02 2.5651000e-03 /

C2H4O(+m)=CH4+CO(+m)                      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -14.63352315265361
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.8098000e+01 -5.6140000e-01 -2.9298000e-01 2.8201000e-02 /
CHEB / 2.2611000e+01 1.2591000e+00 4.8757000e-02 -7.3914000e-02 /
CHEB / -3.2495000e-01 4.3502000e-01 9.4960000e-02 -8.8628000e-03 /
CHEB / -2.3406000e-01 9.2519000e-02 4.3523000e-02 1.0988000e-02 /
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```
C2H3O-1+H(+m)=CH4+CO(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -125.81811010238275
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1512000e+01 -1.2701000e-01 -9.6268000e-02 -5.7771000e-02 /
CHEB / 1.1875000e+00 1.5649000e-01 1.1287000e-01 6.1919000e-02 /
CHEB / 1.2829000e-01 -9.6990000e-03 2.8213000e-04 8.1608000e-03 /
CHEB / 3.0891000e-02 -1.5328000e-02 -1.2153000e-02 -7.9893000e-03 /

C2H3+OH(+m)=CH4+CO(+m)              1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -125.26426138361049 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0137000e+01 -1.3340000e-01 -1.0005000e-01 -5.8982000e-02 /
CHEB / 9.3141000e-01 1.6303000e-01 1.1620000e-01 6.2270000e-02 /
CHEB / 1.2958000e-01 -8.9577000e-03 1.3098000e-03 9.2742000e-03 /
CHEB / 2.9966000e-02 -1.5794000e-02 -1.2290000e-02 -7.8537000e-03 /

C2H3O-2+H(+m)=CH4+CO(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (CH3CHO)  deltaHrxn(T=298K) = -125.81811010238275
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0267000e+01 -1.3999000e-01 -1.0391000e-01 -6.0150000e-02 /
CHEB / 8.4145000e-01 1.6972000e-01 1.1956000e-01 6.2533000e-02 /
CHEB / 1.3110000e-01 -8.1510000e-03 2.3772000e-03 1.0404000e-02 /
CHEB / 3.1537000e-02 -1.6259000e-02 -1.2405000e-02 -7.6820000e-03 /

CH2CHO+H(+m)=CH4+CO(+m)              1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -102.32752533249197 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1160000e+01 -1.7779000e-01 -1.0489000e-01 -4.2329000e-02 /
CHEB / 9.0099000e-01 1.6882000e-01 9.5475000e-02 3.7249000e-02 /
CHEB / 1.7702000e-01 2.5325000e-02 1.7441000e-02 6.3483000e-03 /
CHEB / 5.7473000e-02 -9.0065000e-03 -4.2195000e-03 -1.1990000e-03 /

CH3+HCO(+m)=CH4+CO(+m)              1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -89.37612403080448 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0239000e+01 -8.9487000e-01 -1.4676000e-01 1.6012000e-03 /
CHEB / 1.4023000e+00 8.1367000e-01 8.3295000e-02 -2.0015000e-02 /
CHEB / 1.9334000e-01 1.4300000e-01 5.6015000e-02 1.0264000e-02 /
CHEB / 1.9144000e-02 -3.6076000e-02 8.6917000e-03 5.6358000e-03 /

CH3CO+H(+m)=CH4+CO(+m)              1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3CHO) deltaHrxn(T=298K) = -94.05142144015258 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0189000e+01 -5.7996000e-01 -2.0084000e-01 -1.0524000e-02 /
CHEB / 1.1398000e+00 5.5175000e-01 1.6745000e-01 -8.6539000e-03 /
CHEB / 1.8923000e-01 8.1313000e-02 4.4887000e-02 1.4143000e-02 /
CHEB / 3.4681000e-02 -3.3032000e-02 -4.1411000e-03 5.2178000e-03 /

!PDepNetwork C4H6-13
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     nC4H5             85.18 69.37 18.93 23.55 27.16 29.92 34.02 37.03
      41.81 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     iC4H5             86.31 99.28 18.52 22.6  26.13 29.08 33.64 37.01
      42.26
!Here are the path reactions and their high-P limit kinetics:
!     nC4H5+H=C4H6-13         5.3600000e+14      0.00000
9.8000000e+02
!     C2H3+C2H3=C4H6-13       7.2300000e+13      0.00000
0.0000000e+00
!     iC4H5+H=C4H6-13         1.4157154e+13      -0.15000
2.9166667e+02

nC4H5+H(+m)=C4H6-13(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H6-13) High-P Limit: R_Recombination exact:  Cd_pri_rad     H_rad
      deltaHrxn(T=298K) = -108.31826713346183 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3002000e+01 6.2575000e-01 -5.1133000e-02 /
CHEB / -2.1923000e+00 8.5078000e-01 -8.2035000e-03 /
CHEB / -1.5692000e+00 3.0368000e-01 4.3106000e-02 /
CHEB / -8.1197000e-01 3.1387000e-02 2.2240000e-02 /
CHEB / -3.8835000e-01 -2.4397000e-02 -4.0744000e-04 /

nC4H5+H(+m)=iC4H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H6-13)      deltaHrxn(T=298K) = 1.1298991643721976 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3505000e+01 -8.0624000e-01 -1.0386000e-01 /
CHEB / 1.5130000e+00 9.5840000e-01 8.1583000e-02 /
CHEB / -1.8829000e-01 -2.8218000e-02 5.5943000e-02 /
CHEB / -6.6697000e-02 -1.2090000e-01 -2.0021000e-02 /
CHEB / 2.3601000e-02 -2.6419000e-02 -1.6803000e-02 /

C2H3+C2H3(+m)=C4H6-13(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6-13) High-P Limit: R_Recombination exact:
Cd_pri_rad     Cd_pri_rad           deltaHrxn(T=298K) = -
115.4379729816371 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0906000e+01 2.0810000e+00 -4.3560000e-01 /
CHEB / -3.2213000e+00 8.7132000e-01 2.0638000e-01 /
CHEB / -1.8000000e+00 1.9188000e-01 7.2725000e-02 /
CHEB / -8.4764000e-01 -5.5876000e-03 6.0712000e-03 /
CHEB / -3.9226000e-01 -2.0487000e-02 -3.7262000e-03 /
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```
C2H3+C2H3(+m)=nC4H5+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6-13)      deltaHrxn(T=298K) = -7.119705848175265
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2223000e+00 -3.9836000e-01 -1.5755000e-01 /
CHEB / 4.8885000e-01 5.1487000e-01 1.9011000e-01 /
CHEB / -3.7725000e-02 -7.0902000e-02 -6.2516000e-03 /
CHEB / 2.2993000e-03 -5.9762000e-02 -2.8326000e-02 /
CHEB / 2.0856000e-02 2.8397000e-03 -4.1683000e-03 /

C2H3+C2H3(+m)=iC4H5+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6-13)      deltaHrxn(T=298K) = -5.989806683803074
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3601000e+01 -4.0223000e-01 -1.5324000e-01 /
CHEB / 3.7665000e-01 5.2325000e-01 1.8526000e-01 /
CHEB / -5.8584000e-02 -7.7054000e-02 -6.3848000e-03 /
CHEB / -7.9272000e-03 -5.9160000e-02 -2.7809000e-02 /
CHEB / 1.5566000e-02 4.2709000e-03 -3.9263000e-03 /

iC4H5+H(+m)=C4H6-13(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H6-13) High-P Limit: R_Recombination estimate: (Average:)
Cd_rad/OneDe     H_rad        deltaHrxn(T=298K) = -109.44816629783404
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1148000e+01 6.8539000e-01 -6.6547000e-02 /
CHEB / -2.5408000e+00 8.8597000e-01 -5.4943000e-03 /
CHEB / -1.6207000e+00 3.0165000e-01 4.4985000e-02 /
CHEB / -8.3713000e-01 2.6830000e-02 2.1051000e-02 /
CHEB / -4.0174000e-01 -2.4660000e-02 -1.0310000e-03 /

!PDepNetwork C4H6-12
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78 Primary Thermo Library: CFG (Species ID: CH3CHCCH2)
!     C4H5-113          79.11 71.83 18.91 22.66 25.87 28.57 32.85 36.09
      41.23 Primary Thermo Library: CFG (Species ID: CH3CHCCH)
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96  Primary Thermo Library: CFG (Species ID: H)
!     pC3H3             86.21 60.63 14.9  17.21 19.0  20.43 22.68 24.42
      27.32 Primary Thermo Library: CFG (Species ID: C3H3)
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21 Primary Thermo Library: CFG (Species ID: CH3)
!     CH3CCCH2          72.0  69.45 17.8  21.47 24.86 27.81 32.54 36.07
      42.55 Estimated by Group Additivity
!     iC4H5             86.31 99.28 18.52 22.6  26.13 29.08 33.64 37.01
      42.26 Primary Thermo Library: CFG (Species ID: CH2CHCCH2)
!Here are the path reactions and their high-P limit kinetics:
!     C4H5-113+H=C4H6-12      1.000e+14    0.00        0.00
!     pC3H3+CH3=C4H6-12       2.000e+13    0.00        0.00
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```
!     CH3CCCH2+H=C4H6-12      1.000e+14    0.00        0.00
!     iC4H5+H=C4H6-12         1.000e+14    0.00        0.00

C4H5-113+H(+m)=C4H6-12(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) High-P Limit: R_Recombination Primary
Kinetic Library: Tautomerization    deltaHrxn(T=298K) = -
90.23018059228966 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3073000e+01 6.4690000e-01 -1.7690000e-01 5.6709000e-02 /
CHEB / -1.6663000e+00 7.0693000e-01 -8.3141000e-02 1.1342000e-02 /
CHEB / -9.8459000e-01 2.3267000e-01 2.1408000e-02 -1.6464000e-03 /
CHEB / -4.8685000e-01 2.2962000e-02 2.1688000e-02 2.4063000e-03 /

pC3H3+CH3(+m)=C4H6-12(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) High-P Limit: R_Recombination Primary
Kinetic Library: Tautomerization    deltaHrxn(T=298K) = -
80.48110554107973 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2957000e+01 2.6407000e-01 -5.1584000e-02 1.2951000e-02 /
CHEB / -1.0766000e+00 4.3267000e-01 -7.2850000e-02 1.7353000e-02 /
CHEB / -7.0381000e-01 2.3729000e-01 -2.0960000e-02 5.1834000e-03 /
CHEB / -3.9065000e-01 7.6595000e-02 7.4672000e-03 5.7215000e-04 /

!C4H5-113+H(+m)=pC3H3+CH3(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = -9.749075051209935
kcal/mol
!TCHEB / 300.0 2000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 4   4 /
!CHEB / 1.2371000e+01 -1.1160000e+00 -1.1933000e-01 2.8744000e-02 /
!CHEB / -2.6853000e-01 9.1600000e-01 3.6901000e-02 -2.1794000e-02 /
!CHEB / -6.6715000e-01 1.9934000e-01 7.3499000e-02 -6.4748000e-03 /
!CHEB / -3.8675000e-01 -2.3026000e-02 1.2679000e-02 3.1709000e-03 /

CH3CCCH2+H(+m)=C4H6-12(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) High-P Limit: R_Recombination Primary
Kinetic Library: Tautomerization    deltaHrxn(T=298K) = -
83.12107916649211 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3421000e+01 3.1484000e-01 -6.5354000e-02 1.7479000e-02 /
CHEB / -1.0965000e+00 4.9359000e-01 -8.3017000e-02 2.0022000e-02 /
CHEB / -7.6056000e-01 2.4622000e-01 -1.6013000e-02 4.1780000e-03 /
CHEB / -4.3439000e-01 6.6241000e-02 1.2102000e-02 4.1381000e-04 /

C4H5-113+H(+m)=CH3CCCH2+H(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = -7.10910142579754
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9923000e+00 -1.0871000e+00 -1.1966000e-01 2.7609000e-02 /
CHEB / 1.6336000e-01 9.2778000e-01 4.3848000e-02 -2.3329000e-02 /
CHEB / -5.8034000e-01 1.8697000e-01 7.3983000e-02 -5.5736000e-03 /
CHEB / -3.5210000e-01 -3.0015000e-02 9.4536000e-03 3.5962000e-03 /
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CH3CCCH2+H(+m)=pC3H3+CH3(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = -2.639973625412388
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1703000e+01 -1.3464000e+00 -7.4474000e-02 1.9954000e-02 /
CHEB / 8.8301000e-01 8.7014000e-01 -2.7265000e-02 4.5290000e-03 /
CHEB / -5.3428000e-01 2.6477000e-01 5.6417000e-02 -8.0010000e-03 /
CHEB / -4.4759000e-01 -5.3571000e-05 2.9284000e-02 -2.8716000e-04 /

iC4H5+H(+m)=C4H6-12(+m)                   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) High-P Limit: R_Recombination Primary
Kinetic Library: Tautomerization    deltaHrxn(T=298K) = -
97.42952472083357 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2057000e+01 1.5838000e+00 -4.8629000e-01 1.3086000e-01 /
CHEB / -2.3268000e+00 8.1230000e-01 6.4994000e-02 -4.3304000e-02 /
CHEB / -1.2212000e+00 1.7403000e-01 5.7059000e-02 1.1637000e-03 /
CHEB / -5.3990000e-01 -3.4402000e-03 1.0061000e-02 4.2660000e-03 /

C4H5-113+H(+m)=iC4H5+H(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = 7.199344128543906
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2344000e+01 -6.4258000e-01 -1.6493000e-01 1.1289000e-02 /
CHEB / 2.1823000e+00 7.3703000e-01 1.6229000e-01 -2.6474000e-02 /
CHEB / -3.6588000e-01 -5.6112000e-03 3.3914000e-02 1.6402000e-02 /
CHEB / -1.2391000e-01 -7.8089000e-02 -2.1563000e-02 2.4492000e-03 /

iC4H5+H(+m)=pC3H3+CH3(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = -16.94841917975385
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2516000e+01 -7.0262000e-01 -1.8679000e-01 1.9089000e-02 /
CHEB / -9.7938000e-01 7.4143000e-01 1.6265000e-01 -3.5554000e-02 /
CHEB / -6.6476000e-01 5.2700000e-02 5.0904000e-02 1.3822000e-02 /
CHEB / -2.5592000e-01 -6.5491000e-02 -1.2848000e-02 5.0699000e-03 /

CH3CCCH2+H(+m)=iC4H5+H(+m)                1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6-12) deltaHrxn(T=298K) = 14.308445554341453
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0813000e+01 -6.9363000e-01 -1.8184000e-01 1.7653000e-02 /
CHEB / 3.9522000e+00 7.4379000e-01 1.6253000e-01 -3.3870000e-02 /
CHEB / -5.1818000e-01 4.2648000e-02 4.7685000e-02 1.4375000e-02 /
CHEB / -2.0832000e-01 -6.8927000e-02 -1.4844000e-02 4.6307000e-03 /

!PDepNetwork C4H6-1
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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!     C4H6-1            42.02 69.18 19.47 23.9  27.69 30.86 35.89 39.71
      45.81
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H         137.14      51.64 10.34 10.64 10.89 11.15 11.7  12.22
      13.21
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     pC3H3             86.21 60.63 14.9  17.21 19.0  20.43 22.68 24.42
      27.32
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H5-113          79.11 71.83 18.91 22.66 25.87 28.57 32.85 36.09
      41.23
!     C4H5-114          88.55 72.99 18.78 22.51 25.72 28.43 32.79 36.1
      42.32 null
!Here are the path reactions and their high-P limit kinetics:
!     C2H+C2H5=C4H6-1         1.4157154e+13      -0.15000
2.9166667e+02
!     pC3H3+CH3=C4H6-1        2.4874006e+15      -0.90000
2.5000000e+02
!     C4H5-113+H=C4H6-1             5.0000000e+13      0.00000
0.0000000e+00
!     C4H5-114+H=C4H6-1             1.0000000e+14      0.00000
0.0000000e+00

C2H+C2H5(+m)=C4H6-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#6 (C4H6-1) High-P Limit: R_Recombination estimate: (Average:) Ct_rad
C_rad/H2/Cs       deltaHrxn(T=298K) = -124.53694774318811 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8541000e+00 7.5774000e+00 -7.8528000e-02 /
CHEB / -1.8148000e+00 1.4712000e-01 -1.6035000e-01 /
CHEB / -1.3303000e+00 7.1055000e-02 1.2723000e-02 /
CHEB / -6.7040000e-01 1.2439000e-02 6.8664000e-03 /
CHEB / -3.3576000e-01 -1.0182000e-02 6.3663000e-04 /

C2H+C2H5(+m)=pC3H3+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -45.1056778465256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2738000e+01 -9.2850000e-03 -7.8323000e-03 /
CHEB / -1.3084000e-01 8.5522000e-03 7.2151000e-03 /
CHEB / -5.8589000e-02 3.2912000e-03 2.7578000e-03 /
CHEB / -9.2990000e-03 -1.6662000e-03 -1.3968000e-03 /
CHEB / -1.1317000e-02 -1.1871000e-03 -9.9012000e-04 /

C2H+C2H5(+m)=C4H5-113+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -35.35660279531567 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0726000e+01 -1.8294000e-02 -1.3799000e-02 /
CHEB / 9.5036000e-01 1.6894000e-02 1.2806000e-02 /
CHEB / 2.7833000e-01 5.4069000e-03 4.0433000e-03 /
CHEB / 1.1368000e-01 -2.4370000e-03 -1.8895000e-03 /
CHEB / 3.4777000e-02 -1.8144000e-03 -1.3684000e-03 /
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C2H+C2H5(+m)=C4H5-114+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -25.91750329218116 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0168000e+01 -2.7478000e-02 -1.9711000e-02 /
CHEB / 1.3027000e+00 2.6446000e-02 1.9036000e-02 /
CHEB / 4.3312000e-01 6.6900000e-03 4.7382000e-03 /
CHEB / 1.6797000e-01 -3.7051000e-03 -2.6842000e-03 /
CHEB / 5.0754000e-02 -2.3682000e-03 -1.6870000e-03 /

pC3H3+CH3(+m)=C4H6-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Ct     C_methyl       deltaHrxn(T=298K) = -
79.43126989666251 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2123000e+01 4.2854000e-01 -4.3013000e-02 /
CHEB / -1.4801000e+00 7.2235000e-01 -4.9265000e-02 /
CHEB / -9.8688000e-01 4.4536000e-01 6.8330000e-03 /
CHEB / -5.7038000e-01 1.9841000e-01 3.1869000e-02 /
CHEB / -3.2861000e-01 5.4306000e-02 2.5755000e-02 /

C4H5-113+H(+m)=C4H6-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
89.18034494787244 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2688000e+01 8.7637000e-01 -1.9762000e-01 /
CHEB / -1.5985000e+00 9.6042000e-01 -2.2663000e-02 /
CHEB / -1.0575000e+00 4.6965000e-01 4.4677000e-02 /
CHEB / -6.0400000e-01 1.5608000e-01 4.7438000e-02 /
CHEB / -3.3168000e-01 2.7013000e-02 2.2150000e-02 /

C4H5-113+H(+m)=pC3H3+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -9.749075051209935 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2843000e+01 -1.0242000e+00 -1.5051000e-01 /
CHEB / 8.4812000e-01 9.4240000e-01 6.1093000e-02 /
CHEB / 1.1808000e-01 2.2673000e-01 9.4156000e-02 /
CHEB / -6.8350000e-02 -5.0684000e-02 3.0478000e-02 /
CHEB / -5.2260000e-02 -7.0132000e-02 -1.2936000e-02 /

C4H5-114+H(+m)=C4H6-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -98.61944445100696
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1853000e+01 2.3353000e+00 -6.8790000e-01 /
CHEB / -1.8423000e+00 7.2097000e-01 2.2880000e-01 /
CHEB / -1.2005000e+00 3.8867000e-01 1.0327000e-01 /
CHEB / -6.5590000e-01 1.0617000e-01 4.4555000e-02 /
CHEB / -3.4813000e-01 7.7196000e-03 1.4103000e-02 /
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C4H5-114+H(+m)=pC3H3+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -19.18817455434445 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3691000e+01 -5.8496000e-01 -2.2728000e-01 /
CHEB / 2.6711000e-01 5.5879000e-01 1.9267000e-01 /
CHEB / 3.6813000e-02 1.2176000e-01 6.6336000e-02 /
CHEB / -4.7668000e-02 -4.5367000e-02 -3.5026000e-03 /
CHEB / -4.2379000e-02 -4.3487000e-02 -1.8703000e-02 /

C4H5-114+H(+m)=C4H5-113+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (C4H6-1) deltaHrxn(T=298K) = -9.439099503134521 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1118000e+01 -5.7260000e-01 -2.1234000e-01 /
CHEB / 1.7358000e+00 5.7916000e-01 1.8838000e-01 /
CHEB / 4.5400000e-01 8.8580000e-02 5.7714000e-02 /
CHEB / 7.9580000e-02 -5.7116000e-02 -9.4781000e-03 /
CHEB / 3.0738000e-03 -3.8617000e-02 -1.8927000e-02 /

!PDepNetwork C4H6-2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6-2            34.7  67.78 18.64 22.64 26.42 29.76 35.24 39.38
      47.86 null
!     CH3CCCH2          72.0  69.45 17.8  21.47 24.86 27.81 32.54 36.07
      42.55 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     CH3CCCH2+H=C4H6-2             5.0000000e+13      0.00000
0.0000000e+00

CH3CCCH2+H(+m)=C4H6-2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C4H6-2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Ct     H_rad          deltaHrxn(T=298K) = -
89.39035413596292 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3432000e+01 3.2763000e-01 -3.1887000e-02 /
CHEB / -9.7970000e-01 5.9451000e-01 -4.9559000e-02 /
CHEB / -6.9401000e-01 4.4160000e-01 -1.7275000e-02 /
CHEB / -4.7969000e-01 2.6211000e-01 1.2279000e-02 /
CHEB / -3.0876000e-01 1.1516000e-01 2.5309000e-02 /

!PDepNetwork C4H9-1 + C4H9-2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9-1            20.65 78.53 23.01 28.55 33.6  37.94 44.89 50.17
      58.56
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!     C4H9-2            18.01 78.98 21.99 27.3  32.36 36.82 44.06 49.58
      58.28
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+C2H5=C4H9-1        1.9900000e+03      2.44000
5.3700000e+03
!     C4H8-1+H=C4H9-1         1.1800000e+13      0.00000
3.8000000e+03
!     C4H9-1=C4H9-2                 3.8760000e+10      0.89000
3.5800000e+04
!     C4H9-1=C4H9-2                 2.3600000e+10      0.82000
3.5100000e+04
!     C4H8-1+H=C4H9-2         2.0100000e+13      0.00000
2.1000000e+03
!     C3H6+CH3=C4H9-2         3.1000000e+12      0.00000
8.5000000e+03
!     C4H8-2+H=C4H9-2         1.0000000e+13      0.00000
2.9000000e+03

C4H9-1(+m)=C4H9-2(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) High-P Limit: Summation of kinetics: !intra_H_migration
estimate: (Average:)Others-R2H_S    C_rad_out_2H
Cs_H_out_H/(NonDeC/Cs)
!intra_H_migration exact: Others-R3H_SS    C_rad_out_2H
Cs_H_out_H/NonDeC       deltaHrxn(T=298K) = -2.639603250818574 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.8158000e+00 2.0613000e+00 -5.3257000e-01 /
CHEB / 7.7946000e+00 1.2596000e+00 8.3715000e-02 /
CHEB / -2.8880000e+00 2.5395000e-01 9.0866000e-02 /
CHEB / -1.6327000e+00 -1.8487000e-01 2.1284000e-02 /
CHEB / -7.9300000e-01 -2.3144000e-01 -3.0216000e-02 /

C2H4+C2H5(+m)=C4H9-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H2     C_rad/H2/Cs         deltaHrxn(T=298K) = -
22.3278384868145 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4628000e+00 6.4012000e-01 -5.0428000e-02 /
CHEB / 3.5588000e-02 1.0071000e+00 -3.7537000e-02 /
CHEB / -1.8030000e+00 4.6696000e-01 4.6563000e-02 /
CHEB / -1.1798000e+00 4.9002000e-02 5.6249000e-02 /
CHEB / -6.3164000e-01 -1.1543000e-01 1.3349000e-02 /
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C2H4+C2H5(+m)=C4H9-2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -24.967441737633074 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8038000e+00 6.5125000e-01 -4.6816000e-01 /
CHEB / 3.2976000e+00 1.9088000e+00 1.9821000e-01 /
CHEB / -1.6658000e+00 4.4728000e-01 1.5195000e-01 /
CHEB / -1.1250000e+00 -1.0988000e-01 4.1800000e-02 /
CHEB / -5.8687000e-01 -1.6959000e-01 -2.0168000e-02 /

C2H4+C2H5(+m)=C3H6+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -1.4902041559760661 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1124000e+00 -1.5370000e+00 -2.9288000e-01 /
CHEB / 6.8810000e+00 1.6657000e+00 2.1875000e-01 /
CHEB / 1.9936000e-01 1.3925000e-01 1.3538000e-01 /
CHEB / -1.0866000e-01 -1.8574000e-01 -9.4132000e-04 /
CHEB / -4.1345000e-02 -1.0311000e-01 -4.3012000e-02 /

C4H8-1+H(+m)=C4H9-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H/Nd_Cd/H2
H_rad       deltaHrxn(T=298K) = -33.32622846571959 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4312000e+00 1.2640000e+00 -2.3788000e-01 /
CHEB / -2.3733000e+00 1.5594000e+00 -7.8682000e-02 /
CHEB / -2.3730000e+00 5.3461000e-01 1.0849000e-01 /
CHEB / -1.3470000e+00 -3.2476000e-03 7.7944000e-02 /
CHEB / -6.7166000e-01 -1.4279000e-01 3.1806000e-03 /

C4H8-1+H(+m)=C4H9-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H/Nd
H_rad       deltaHrxn(T=298K) = -35.96583171653816 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9793000e+00 1.6132000e+00 -3.4908000e-01 /
CHEB / -2.6787000e+00 9.7555000e-01 1.7464000e-01 /
CHEB / -2.1355000e+00 2.7763000e-01 9.8570000e-02 /
CHEB / -1.1571000e+00 -4.2665000e-02 2.1253000e-02 /
CHEB / -5.6110000e-01 -9.6986000e-02 -1.4650000e-02 /

C4H8-1+H(+m)=C2H4+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -10.998389978905092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0639000e+01 -1.0265000e+00 -1.3556000e-01 /
CHEB / 2.1544000e+00 1.0446000e+00 4.5044000e-02 /
CHEB / -1.4004000e-02 1.8236000e-01 1.2175000e-01 /
CHEB / -1.1463000e-01 -1.1577000e-01 2.5765000e-02 /
CHEB / -4.2643000e-02 -9.5177000e-02 -3.5512000e-02 /

C4H8-1+H(+m)=C3H6+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -12.488594134881154 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.2085000e+01 -6.3050000e-01 -1.8644000e-01 /
CHEB / 1.2066000e+00 7.2032000e-01 1.7858000e-01 /
CHEB / 8.2969000e-03 2.1781000e-02 5.0764000e-02 /
CHEB / -4.7128000e-02 -9.7668000e-02 -2.3676000e-02 /
CHEB / -5.0784000e-03 -3.4121000e-02 -2.3126000e-02 /

C4H8-1+H(+m)=C4H8-2+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -2.719803185470056 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9310000e+00 -5.8576000e-01 -1.8166000e-01 /
CHEB / 2.3046000e+00 6.8754000e-01 1.8032000e-01 /
CHEB / 2.6422000e-01 -6.9094000e-03 4.3290000e-02 /
CHEB / 2.5564000e-02 -8.8208000e-02 -2.7044000e-02 /
CHEB / 2.1570000e-02 -2.4816000e-02 -2.0445000e-02 /

C3H6+CH3(+m)=C4H9-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) deltaHrxn(T=298K) = -20.837634330838434 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6020000e+00 5.1737000e-01 -3.8267000e-01 /
CHEB / 2.8662000e+00 2.1439000e+00 1.0091000e-01 /
CHEB / -2.0539000e+00 5.3866000e-01 1.3614000e-01 /
CHEB / -1.3000000e+00 -9.0230000e-02 4.7359000e-02 /
CHEB / -6.5488000e-01 -1.7482000e-01 -1.6657000e-02 /

C3H6+CH3(+m)=C4H9-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H/Nd
C_methyl          deltaHrxn(T=298K) = -23.477237581657008 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1604000e+00 8.2587000e-01 -9.2596000e-02 /
CHEB / -1.4831000e-01 9.8838000e-01 2.6935000e-02 /
CHEB / -2.0370000e+00 3.2864000e-01 6.8337000e-02 /
CHEB / -1.1332000e+00 -1.6331000e-02 2.8348000e-02 /
CHEB / -5.6363000e-01 -9.3680000e-02 -9.3026000e-03 /

C4H8-2+H(+m)=C4H9-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) deltaHrxn(T=298K) = -30.606425280249532 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7761000e+00 6.8466000e-01 -3.9493000e-01 /
CHEB / 7.7190000e-02 2.2764000e+00 9.3628000e-02 /
CHEB / -2.0566000e+00 5.3380000e-01 1.4551000e-01 /
CHEB / -1.3212000e+00 -9.9497000e-02 5.0755000e-02 /
CHEB / -6.5900000e-01 -1.7689000e-01 -1.6815000e-02 /

C4H8-2+H(+m)=C4H9-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H9-1) High-P Limit: R_Addition_MultipleBond estimate: (Average:)
Cd/H/Nd_Cd/H/Nd     H_rad           deltaHrxn(T=298K) = -
33.246028531068106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5522000e+00 1.2886000e+00 -2.4972000e-01 /
CHEB / -2.2760000e+00 1.0082000e+00 1.1453000e-01 /
CHEB / -2.1119000e+00 2.9600000e-01 8.7107000e-02 /
CHEB / -1.1551000e+00 -3.7100000e-02 2.3055000e-02 /
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CHEB / -5.6485000e-01 -9.7360000e-02 -1.3339000e-02 /

C4H8-2+H(+m)=C2H4+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -8.278586793435036 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0684000e+00 -1.4752000e+00 -2.9275000e-01 /
CHEB / 4.6325000e+00 1.6301000e+00 2.2455000e-01 /
CHEB / 2.3854000e-01 9.6123000e-02 1.3387000e-01 /
CHEB / -8.9759000e-02 -1.8411000e-01 -8.4469000e-03 /
CHEB / -3.2097000e-02 -9.2287000e-02 -4.4942000e-02 /

C4H8-2+H(+m)=C3H6+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9-1) deltaHrxn(T=298K) = -9.768790949411098 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1261000e+01 -7.1781000e-01 -1.7027000e-01 /
CHEB / 1.6239000e+00 8.1783000e-01 1.4982000e-01 /
CHEB / -2.5546000e-02 2.6864000e-02 6.3338000e-02 /
CHEB / -7.4446000e-02 -1.0905000e-01 -1.9466000e-02 /
CHEB / -1.4682000e-02 -4.0252000e-02 -2.5973000e-02 /

!PDepNetwork iC4H9 + tC4H9
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H9             19.15 76.39 23.23 28.98 34.04 38.33 45.13 50.31
      58.58
!     tC4H9             14.3  76.21 21.71 26.64 31.62 36.12 43.55 49.22
      58.13
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     C3H6+CH3=iC4H9          1.3600000e+12      0.00000
1.0100000e+04
!     iC4H8+H=iC4H9           1.1700000e+13      0.00000
4.7000000e+03
!     iC4H9=tC4H9                   6.2339791e+09      0.93630
3.7689907e+04
!     iC4H8+H=tC4H9           4.9400000e+13      0.00000
1.5000000e+03

iC4H9(+m)=tC4H9(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (iC4H9) High-P Limit: intra_H_migration estimate: (Average:) Others-
R2H_S    C_rad_out_2H     Cs_H_out        deltaHrxn(T=298K) = -
4.849350664026865 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0306000e+00 1.2649000e+00 -2.0979000e-01 /
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CHEB / 8.2463000e+00 1.2748000e+00 2.3786000e-02 /
CHEB / -3.2240000e+00 3.0416000e-01 8.8270000e-02 /
CHEB / -1.9123000e+00 -1.7299000e-01 3.3755000e-02 /
CHEB / -9.6157000e-01 -2.6423000e-01 -2.3311000e-02 /

C3H6+CH3(+m)=iC4H9(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (iC4H9) High-P Limit: R_Addition_MultipleBond exact:  Cd/H/Nd_Cd/H2
C_methyl          deltaHrxn(T=298K) = -22.3374994328185 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0285000e+00 7.6594000e-01 -6.3047000e-02 /
CHEB / -2.6732000e-02 1.0554000e+00 -4.9926000e-03 /
CHEB / -2.3683000e+00 3.7111000e-01 6.6169000e-02 /
CHEB / -1.3573000e+00 -1.9593000e-02 3.7503000e-02 /
CHEB / -6.7268000e-01 -1.1587000e-01 -5.8724000e-03 /

C3H6+CH3(+m)=tC4H9(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (iC4H9)  deltaHrxn(T=298K) = -27.186850096845365 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1568000e+00 9.2989000e-02 -2.4468000e-01 /
CHEB / 3.5054000e+00 2.2362000e+00 4.8288000e-02 /
CHEB / -2.1642000e+00 6.7623000e-01 1.2314000e-01 /
CHEB / -1.4684000e+00 -1.3828000e-02 5.5072000e-02 /
CHEB / -7.7084000e-01 -1.7386000e-01 -4.8607000e-03 /

iC4H8+H(+m)=iC4H9(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (iC4H9) High-P Limit: R_Addition_MultipleBond exact:  Cd/Nd2_Cd/H2
H_rad       deltaHrxn(T=298K) = -30.726446445329447 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9929000e+00 9.4775000e-01 -1.1089000e-01 /
CHEB / -1.9315000e+00 1.1578000e+00 9.2348000e-03 /
CHEB / -2.3706000e+00 3.7603000e-01 7.8966000e-02 /
CHEB / -1.3425000e+00 -2.1815000e-02 3.6385000e-02 /
CHEB / -6.5838000e-01 -1.1280000e-01 -8.3059000e-03 /

iC4H8+H(+m)=tC4H9(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (iC4H9) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/Nd2
H_rad       deltaHrxn(T=298K) = -35.575797109356316 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1692000e+01 5.9652000e-01 -3.3629000e-02 /
CHEB / -2.4235000e+00 9.9417000e-01 -3.1325000e-02 /
CHEB / -2.1645000e+00 5.4549000e-01 3.1245000e-02 /
CHEB / -1.3848000e+00 1.2700000e-01 5.2859000e-02 /
CHEB / -7.6185000e-01 -9.6407000e-02 2.4184000e-02 /

iC4H8+H(+m)=C3H6+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (iC4H9)  deltaHrxn(T=298K) = -8.388947012510947 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0375000e+01 -8.6383000e-01 -1.3594000e-01 /
CHEB / 2.7078000e+00 9.5869000e-01 8.9322000e-02 /
CHEB / 1.1830000e-02 5.6810000e-02 8.5607000e-02 /
CHEB / -5.7413000e-02 -1.1811000e-01 -7.8175000e-03 /
CHEB / -1.5440000e-03 -5.2767000e-02 -2.7768000e-02 /
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!PDepNetwork C4H7-11 + C4H7-12 + C4H7-24 + C4H7-14 + C4H7-22
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7-11           58.99 75.0  20.38 25.34 29.68 33.36 39.14 43.48
      50.22 null
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C4H7-12           56.79 75.42 20.23 24.88 29.1  32.76 38.62 43.06
      49.99 null
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     C2H2              56.1  47.73 10.27 11.79 12.85 13.67 14.94 15.97
      17.79
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H6-1            42.02 69.18 19.47 23.9  27.69 30.86 35.89 39.71
      45.81
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     pC3H4             46.16 58.99 14.37 17.14 19.55 21.6  24.93 27.49
      31.65
!     C4H6-2            34.7  67.78 18.64 22.64 26.42 29.76 35.24 39.38
      47.86 null
!Here are the path reactions and their high-P limit kinetics:
!     C2H2+C2H5=C4H7-11       2.5050000e+10      0.00000
6.9900000e+03
!     C4H6-1+H=C4H7-11        5.7700000e+13      0.00000
5.3000000e+03
!     C4H7-11=C4H7-24              3.6920000e+10      0.74000
3.4700000e+04
!     C4H6-12+H=C4H7-24            1.2800000e+13      0.00000
3.7000000e+03
!     C4H6-13+H=C4H7-24            3.7100000e+13      0.00000
1.0000000e+03
!     C4H7-12=C4H7-24              2.8960000e+10      0.82000
3.7500000e+04
!     C4H6-1+H=C4H7-12        1.1200000e+14      0.00000
3.7000000e+03
!     aC3H4+CH3=C4H7-12       9.2300000e+12      0.00000
9.4000000e+03
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!     C4H6-12+H=C4H7-12             1.0000000e+13      0.00000
2.9000000e+03
!     C4H7-11=C4H7-12               3.2400000e+11      0.73000
4.2400000e+04
!     C4H7-12=C4H7-14               6.9120000e+09      1.24000
3.6300000e+04
!     C2H3+C2H4=C4H7-14       2.0900000e+13      0.00000
5.2000000e+03
!     C4H6-13+H=C4H7-14             2.8500000e+13      0.00000
4.3000000e+03
!     C4H7-14=C4H7-24               5.6400000e+08      1.28000
2.7900000e+04
!     C4H7-11=C4H7-14               1.8288499e+09      1.13906
3.4790987e+04
!     C4H7-22=C4H7-24               2.3220000e+10      1.08000
3.8700000e+04
!     C4H7-22=C4H7-24               2.1960000e+10      1.12000
4.1300000e+04
!     C4H6-12+H=C4H7-22             6.6800000e+13      0.00000
2.9000000e+03
!     pC3H4+CH3=C4H7-22       1.3200000e+14      0.00000
1.0300000e+04
!     C4H6-2+H=C4H7-22        5.0039096e+13      0.00000
4.1000000e+03

C4H7-11(+m)=C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration exact:  R3H_DS
Cd_rad_out_singleH     Cs_H_out_H/NonDeC        deltaHrxn(T=298K) = -
24.207486076651136 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5103000e+00 1.0421000e+00 -1.9984000e-01 /
CHEB / 8.9301000e+00 1.3993000e+00 -1.1986000e-01 /
CHEB / -2.1586000e+00 5.9914000e-01 3.0131000e-02 /
CHEB / -1.3649000e+00 9.0443000e-02 4.2773000e-02 /
CHEB / -7.6874000e-01 -1.1369000e-01 7.7648000e-03 /

C4H7-11(+m)=C4H7-12(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration exact:  R2H_D
Cd_rad_out_singleH     Cd_H_out_singleNd        deltaHrxn(T=298K) = -
2.1997755775516623 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0853000e+00 1.6874000e+00 2.5194000e-02 /
CHEB / 1.0424000e+01 1.4879000e+00 -1.1039000e-01 /
CHEB / -2.2100000e+00 3.7379000e-02 5.6757000e-02 /
CHEB / -1.2996000e+00 -9.2715000e-02 8.3125000e-03 /
CHEB / -6.5619000e-01 -1.3168000e-01 -2.3237000e-02 /

C4H7-11(+m)=C4H7-14(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration estimate: (Average:)
R4H_DSS     Cd_rad_out_singleH     Cs_H_out_2H        deltaHrxn(T=298K)
= -10.0989013019461 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1802000e+00 1.1967000e+00 -2.1591000e-01 /
CHEB / 8.3876000e+00 1.4505000e+00 -9.3215000e-02 /
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CHEB / -2.5617000e+00 5.4199000e-01 4.5216000e-02 /
CHEB / -1.5735000e+00 1.2226000e-02 4.1428000e-02 /
CHEB / -8.4227000e-01 -1.6337000e-01 -2.6191000e-03 /

C4H7-11(+m)=C4H7-22(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11)      deltaHrxn(T=298K) = -5.3095156360373394 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.4443000e+00 6.0610000e-01 -2.9349000e-01 /
CHEB / 1.0389000e+01 1.8763000e+00 1.0819000e-01 /
CHEB / -1.8709000e+00 4.2409000e-01 5.2475000e-02 /
CHEB / -1.2325000e+00 -3.3149000e-02 1.7911000e-02 /
CHEB / -6.5834000e-01 -1.3090000e-01 -2.0360000e-03 /

C4H7-12(+m)=C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    Cd_rad_out_double     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -22.007710499099474 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.3645000e+00 9.0628000e-01 -2.5832000e-01 /
CHEB / 9.6778000e+00 1.6262000e+00 -1.1296000e-01 /
CHEB / -2.1310000e+00 5.3243000e-01 8.6634000e-02 /
CHEB / -1.2867000e+00 2.6273000e-02 4.3290000e-02 /
CHEB / -6.9674000e-01 -1.2425000e-01 -1.2295000e-02 /

C4H7-12(+m)=C4H7-14(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration exact:  Others-R3H_SS
Cd_rad_out_double     Cs_H_out_2H         deltaHrxn(T=298K) = -
7.8991257243944375 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.4453000e+00 1.6347000e+00 -3.3362000e-01 /
CHEB / 8.5725000e+00 1.2481000e+00 8.1758000e-02 /
CHEB / -2.5768000e+00 3.3132000e-01 4.6983000e-02 /
CHEB / -1.4876000e+00 -6.5274000e-02 -6.6308000e-03 /
CHEB / -7.4858000e-01 -1.4501000e-01 -2.7733000e-02 /

C4H7-12(+m)=C4H7-22(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11)      deltaHrxn(T=298K) = -3.109740058485677 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3480000e+00 5.8556000e-01 -3.0432000e-01 /
CHEB / 1.1117000e+01 1.9481000e+00 7.5094000e-02 /
CHEB / -1.8189000e+00 3.9551000e-01 8.5925000e-02 /
CHEB / -1.1448000e+00 -6.9297000e-02 2.5581000e-02 /
CHEB / -5.9006000e-01 -1.3881000e-01 -1.2932000e-02 /

C4H7-14(+m)=C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: intra_H_migration exact:  Others-R2H_S
C_rad_out_2H     Cs_H_out_H/OneDe         deltaHrxn(T=298K) = -
14.108584774705037 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.4661000e-01 6.3256000e-01 -4.6838000e-02 /
CHEB / 6.9661000e+00 1.0060000e+00 -3.8560000e-02 /
CHEB / -2.1610000e+00 4.6796000e-01 4.2459000e-02 /
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CHEB / -1.4077000e+00 2.7607000e-02 5.6968000e-02 /
CHEB / -7.6915000e-01 -1.6033000e-01 1.5836000e-02 /

C4H7-22(+m)=C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11) High-P Limit: Summation of kinetics: !intra_H_migration
exact: R3H_DS     Cd_rad_out_singleNd     Cs_H_out_2H
!intra_H_migration exact: Others-R2H_S    Cd_rad_out_double
Cs_H_out_2H       deltaHrxn(T=298K) = -18.897970440613797 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0524000e+00 1.4643000e+00 -2.8158000e-01 /
CHEB / 9.9277000e+00 1.0917000e+00 3.6905000e-02 /
CHEB / -2.1504000e+00 3.1523000e-01 1.2498000e-02 /
CHEB / -1.2254000e+00 1.4171000e-02 -1.4460000e-02 /
CHEB / -6.3069000e-01 -6.2598000e-02 -1.2342000e-02 /

C4H7-22(+m)=C4H7-14(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H7-11)      deltaHrxn(T=298K) = -4.78938566590876 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5570000e+00 5.9220000e-01 -4.6087000e-01 /
CHEB / 1.0182000e+01 2.0316000e+00 1.0664000e-01 /
CHEB / -2.4757000e+00 4.3130000e-01 1.1582000e-01 /
CHEB / -1.4663000e+00 -8.8382000e-02 1.0576000e-02 /
CHEB / -7.3602000e-01 -1.5760000e-01 -3.0171000e-02 /

C2H2+C2H5(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Ct/H_Ct/H     C_rad/H2/Cs           deltaHrxn(T=298K) = -
26.537009675982205 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2994000e+00 5.6678000e-01 -4.6203000e-02 /
CHEB / 2.0030000e-01 9.0624000e-01 -3.4452000e-02 /
CHEB / -1.6358000e+00 4.7030000e-01 3.5334000e-02 /
CHEB / -1.0172000e+00 1.1341000e-01 4.8223000e-02 /
CHEB / -5.6760000e-01 -5.8410000e-02 1.8932000e-02 /

C2H2+C2H5(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -50.74449575263334
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4703000e+00 -1.1461000e-01 -2.9953000e-01 /
CHEB / 2.1817000e+00 2.3209000e+00 -9.4120000e-02 /
CHEB / -1.5263000e+00 8.3946000e-01 1.0040000e-01 /
CHEB / -1.1562000e+00 1.5062000e-01 4.9770000e-02 /
CHEB / -6.6563000e-01 -5.9478000e-02 1.8903000e-03 /

C2H2+C2H5(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -28.736785253533867
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5424000e-01 9.0911000e-01 -1.5911000e-01 /
CHEB / 3.1670000e+00 1.7957000e+00 9.2941000e-03 /
CHEB / -1.5492000e+00 2.8854000e-01 9.6617000e-02 /
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CHEB / -1.0061000e+00 2.4411000e-02 -4.5837000e-03 /
CHEB / -5.3260000e-01 -6.7824000e-02 -1.2122000e-02 /

C2H2+C2H5(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -36.635910977928305
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7768000e+00 2.7798000e-02 -3.0120000e-01 /
CHEB / 1.6467000e+00 2.3557000e+00 -8.9646000e-02 /
CHEB / -1.9148000e+00 8.0168000e-01 1.0829000e-01 /
CHEB / -1.3605000e+00 8.5688000e-02 6.1810000e-02 /
CHEB / -7.4251000e-01 -1.1208000e-01 -3.1253000e-03 /

C2H2+C2H5(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -31.846525312019544
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2784000e+00 -3.2653000e-01 -3.4492000e-01 /
CHEB / 3.4501000e+00 2.5530000e+00 9.9957000e-02 /
CHEB / -1.2582000e+00 6.2080000e-01 9.1782000e-02 /
CHEB / -9.7991000e-01 7.8485000e-02 3.6931000e-02 /
CHEB / -5.4642000e-01 -6.4118000e-02 3.5952000e-03 /

C2H2+C2H5(+m)=C4H6-13+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -4.479630833718609
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7083000e+00 -2.0994000e+00 -2.2834000e-01 /
CHEB / 5.4867000e+00 2.0297000e+00 7.7521000e-02 /
CHEB / -3.1163000e-02 3.9748000e-01 1.8257000e-01 /
CHEB / -2.8119000e-01 -1.3741000e-01 3.7181000e-02 /
CHEB / -1.1321000e-01 -1.4767000e-01 -3.3735000e-02 /

C2H2+C2H5(+m)=aC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -3.1698103507032798
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3240000e+00 -1.2505000e+00 -2.6401000e-01 /
CHEB / 6.3729000e+00 1.2988000e+00 2.0870000e-01 /
CHEB / -8.0683000e-02 1.5601000e-01 9.4872000e-02 /
CHEB / -1.8696000e-01 -1.1199000e-01 5.8834000e-03 /
CHEB / -7.6998000e-02 -8.8493000e-02 -2.2816000e-02 /

C2H2+C2H5(+m)=C2H3+C2H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = 0.2202688633635379
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5544000e+00 -1.8761000e+00 -2.2512000e-01 /
CHEB / 5.3175000e+00 1.8581000e+00 1.0295000e-01 /
CHEB / -8.7897000e-02 3.2010000e-01 1.4816000e-01 /
CHEB / -2.6246000e-01 -1.3645000e-01 3.9572000e-02 /
CHEB / -9.6490000e-02 -1.3763000e-01 -2.6803000e-02 /
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C2H2+C2H5(+m)=pC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -4.119789057522581
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9857000e+00 -2.0591000e+00 -3.1674000e-01 /
CHEB / 6.7533000e+00 2.1787000e+00 2.1036000e-01 /
CHEB / 1.6830000e-01 1.9483000e-01 1.5989000e-01 /
CHEB / -1.6453000e-01 -1.8202000e-01 1.5856000e-02 /
CHEB / -5.9119000e-02 -1.2959000e-01 -4.2806000e-02 /

C4H6-1+H(+m)=C4H7-11(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Ct/Nd_Ct/H     H_rad          deltaHrxn(T=298K) = -35.12585606368127
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0031000e+01 9.4189000e-01 -1.6192000e-01 /
CHEB / -8.7009000e-01 1.2153000e+00 -4.6172000e-02 /
CHEB / -1.8506000e+00 5.4199000e-01 5.8838000e-02 /
CHEB / -1.0956000e+00 9.7475000e-02 5.7505000e-02 /
CHEB / -5.8560000e-01 -7.3887000e-02 1.3047000e-02 /

C4H6-1+H(+m)=C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -59.333342140332405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1756000e+00 6.7808000e-01 -5.2251000e-01 /
CHEB / 2.7049000e-01 2.2449000e+00 5.9376000e-02 /
CHEB / -1.5981000e+00 8.1033000e-01 8.4593000e-02 /
CHEB / -1.1261000e+00 1.5099000e-01 2.7879000e-02 /
CHEB / -6.3363000e-01 -4.6431000e-02 1.8697000e-03 /

C4H6-1+H(+m)=C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Ct/H_Ct/Nd     H_rad          deltaHrxn(T=298K) = -37.32563164123293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7770000e+00 2.0640000e+00 -4.4041000e-01 /
CHEB / -1.7577000e+00 7.6437000e-01 2.3109000e-01 /
CHEB / -1.8451000e+00 2.0491000e-01 9.3051000e-02 /
CHEB / -9.6381000e-01 -3.0187000e-02 1.2718000e-02 /
CHEB / -4.6358000e-01 -6.4233000e-02 -1.2482000e-02 /

C4H6-1+H(+m)=C4H7-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -45.22475736562737
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8036000e+00 1.2088000e+00 -5.1655000e-01 /
CHEB / -6.0669000e-01 1.9072000e+00 1.2706000e-01 /
CHEB / -2.0153000e+00 6.9202000e-01 1.6940000e-02 /
CHEB / -1.2986000e+00 1.1310000e-01 1.4781000e-02 /
CHEB / -6.9094000e-01 -6.3715000e-02 1.4338000e-02 /
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C4H6-1+H(+m)=C4H7-22(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -40.43537169971861
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4981000e+00 5.6010000e-01 -5.2733000e-01 /
CHEB / 1.4304000e+00 2.3264000e+00 2.0487000e-01 /
CHEB / -1.2831000e+00 6.4169000e-01 7.9091000e-02 /
CHEB / -9.4907000e-01 8.3793000e-02 2.8307000e-02 /
CHEB / -5.1795000e-01 -5.7658000e-02 3.2194000e-03 /

C4H6-1+H(+m)=C2H2+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -8.58884638769906
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0078000e+01 -1.0793000e+00 -1.2602000e-01 /
CHEB / 2.0990000e+00 1.0265000e+00 3.4447000e-02 /
CHEB / -2.5275000e-01 2.5031000e-01 1.0510000e-01 /
CHEB / -2.4091000e-01 -8.0834000e-02 3.8477000e-02 /
CHEB / -9.9758000e-02 -1.0149000e-01 -2.1162000e-02 /

C4H6-1+H(+m)=C4H6-12+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -1.0498356444172146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3081000e+00 -4.3565000e-01 -1.7169000e-01 /
CHEB / 2.5952000e+00 5.2072000e-01 1.8804000e-01 /
CHEB / 2.3642000e-01 -2.1526000e-02 1.5879000e-02 /
CHEB / 3.9379000e-02 -6.3347000e-02 -2.6177000e-02 /
CHEB / 2.1404000e-02 -1.1548000e-02 -1.1128000e-02 /

C4H6-1+H(+m)=C4H6-13+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -13.068477221417673
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9271000e+00 -1.5526000e+00 -2.8731000e-01 /
CHEB / 3.6993000e+00 1.5558000e+00 1.9660000e-01 /
CHEB / 1.4487000e-01 2.5818000e-01 1.2886000e-01 /
CHEB / -1.2805000e-01 -1.3041000e-01 2.4454000e-02 /
CHEB / -4.5752000e-02 -1.1577000e-01 -3.1138000e-02 /

C4H6-1+H(+m)=aC3H4+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -11.758656738402344
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2252000e+01 -4.6391000e-01 -1.8449000e-01 /
CHEB / 1.5616000e+00 5.4040000e-01 1.9676000e-01 /
CHEB / -2.9504000e-02 1.5083000e-03 2.4585000e-02 /
CHEB / -4.1174000e-02 -7.2582000e-02 -2.7132000e-02 /
CHEB / -7.1398000e-03 -2.0346000e-02 -1.5083000e-02 /
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C4H6-1+H(+m)=C2H3+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -8.368577524335526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0143000e+01 -1.1427000e+00 -2.8290000e-01 /
CHEB / 3.2295000e+00 1.1706000e+00 2.6984000e-01 /
CHEB / 1.3236000e-01 1.4971000e-01 3.2830000e-02 /
CHEB / -9.1059000e-02 -8.7895000e-02 1.1229000e-02 /
CHEB / -2.7053000e-02 -7.5502000e-02 -5.0158000e-03 /

C4H6-1+H(+m)=pC3H4+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -12.708635445221645
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2965000e+00 -1.6502000e+00 -3.3240000e-01 /
CHEB / 4.9083000e+00 1.7794000e+00 2.6139000e-01 /
CHEB / 3.6895000e-01 1.3370000e-01 1.2765000e-01 /
CHEB / -5.1304000e-02 -1.6972000e-01 5.7396000e-03 /
CHEB / -1.1233000e-02 -1.0524000e-01 -4.4348000e-02 /

C4H6-1+H(+m)=C4H6-2+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -7.319110613888014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6804000e+00 -1.6735000e+00 -3.3651000e-01 /
CHEB / 5.2558000e+00 1.7913000e+00 2.6495000e-01 /
CHEB / 4.6874000e-01 1.4867000e-01 1.2574000e-01 /
CHEB / -1.7106000e-02 -1.6664000e-01 8.6993000e-03 /
CHEB / 1.4639000e-03 -1.0798000e-01 -4.2593000e-02 /

C4H6-12+H(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -34.076020419264054
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1187000e+00 1.2898000e-01 -2.6138000e-01 /
CHEB / 7.7667000e-01 2.2615000e+00 3.6557000e-02 /
CHEB / -1.5170000e+00 5.7244000e-01 1.2847000e-01 /
CHEB / -1.0933000e+00 -5.2437000e-03 4.0008000e-02 /
CHEB / -5.7750000e-01 -9.6677000e-02 -1.2627000e-02 /

C4H6-12+H(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Ca_Cd/H/Nd     H_rad          deltaHrxn(T=298K) = -58.28350649591519
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7974000e+00 1.4219000e+00 -3.3384000e-01 /
CHEB / -1.5444000e+00 1.4608000e+00 -6.4993000e-02 /
CHEB / -1.7646000e+00 5.8246000e-01 4.9920000e-02 /
CHEB / -1.0224000e+00 1.5686000e-01 2.8514000e-02 /
CHEB / -5.6008000e-01 -1.3809000e-02 9.3857000e-03 /
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C4H6-12+H(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/Nd_Ca     H_rad          deltaHrxn(T=298K) = -36.27579599681572
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4907000e+00 1.5933000e+00 -3.3466000e-01 /
CHEB / -1.9724000e+00 8.6011000e-01 1.7489000e-01 /
CHEB / -1.8164000e+00 2.4194000e-01 8.4875000e-02 /
CHEB / -9.6148000e-01 -1.9762000e-02 1.5329000e-02 /
CHEB / -4.6546000e-01 -6.3002000e-02 -1.0994000e-02 /

C4H6-12+H(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -44.174921721210154
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5162000e+00 7.6789000e-01 -5.4220000e-01 /
CHEB / -1.4221000e+00 2.3354000e+00 8.9136000e-02 /
CHEB / -2.1468000e+00 6.2194000e-01 1.5915000e-01 /
CHEB / -1.2870000e+00 4.9102000e-03 2.6020000e-02 /
CHEB / -6.6206000e-01 -1.1236000e-01 -2.5816000e-02 /

C4H6-12+H(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Ca     H_rad      deltaHrxn(T=298K) = -39.385536055301394 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6302000e+00 2.0541000e+00 -3.1788000e-01 /
CHEB / -2.3809000e+00 6.0563000e-01 2.1085000e-01 /
CHEB / -1.8883000e+00 1.0893000e-01 5.6046000e-02 /
CHEB / -9.4567000e-01 -3.3937000e-02 -2.7731000e-03 /
CHEB / -4.3586000e-01 -3.9292000e-02 -1.0859000e-02 /

C4H6-12+H(+m)=C2H2+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -7.539010743281846
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3320000e+00 -1.7192000e+00 -2.4661000e-01 /
CHEB / 3.9024000e+00 1.8651000e+00 1.4235000e-01 /
CHEB / 4.7699000e-03 1.2485000e-01 1.5977000e-01 /
CHEB / -1.9617000e-01 -1.7778000e-01 7.6774000e-03 /
CHEB / -6.8336000e-02 -1.0290000e-01 -4.2373000e-02 /

C4H6-12+H(+m)=C4H6-13+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -12.018641577000459
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0261000e+01 -9.3973000e-01 -1.6986000e-01 /
CHEB / 2.0785000e+00 9.5445000e-01 9.2320000e-02 /
CHEB / 8.7897000e-02 1.5092000e-01 1.1304000e-01 /
CHEB / -4.0159000e-02 -9.1170000e-02 1.1371000e-02 /
CHEB / -2.1022000e-02 -7.5315000e-02 -3.0734000e-02 /
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C4H6-12+H(+m)=aC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -10.70882109398513
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1442000e+01 -5.6756000e-01 -1.8134000e-01 /
CHEB / 1.3875000e+00 6.5929000e-01 1.8299000e-01 /
CHEB / -4.0386000e-02 2.5437000e-03 3.7511000e-02 /
CHEB / -5.8699000e-02 -8.5732000e-02 -2.5278000e-02 /
CHEB / -1.1414000e-02 -2.5797000e-02 -1.8356000e-02 /

C4H6-12+H(+m)=C2H3+C2H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -7.318741879918312
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0437000e+01 -1.4666000e+00 -3.2827000e-01 /
CHEB / 2.5435000e+00 1.6211000e+00 2.6480000e-01 /
CHEB / -1.6786000e-02 8.2932000e-02 1.3641000e-01 /
CHEB / -1.1546000e-01 -1.7950000e-01 -2.1396000e-02 /
CHEB / -2.9968000e-02 -7.8200000e-02 -4.4657000e-02 /

C4H6-12+H(+m)=pC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -11.658799800804431
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2587000e+01 -3.0730000e-01 -1.4010000e-01 /
CHEB / 1.1450000e+00 3.9220000e-01 1.7039000e-01 /
CHEB / -1.9606000e-02 -4.7128000e-02 -8.1929000e-03 /
CHEB / -3.8011000e-04 -4.6140000e-02 -2.3463000e-02 /
CHEB / 1.9608000e-02 -1.6209000e-03 -4.0641000e-03 /

C4H6-12+H(+m)=C4H6-2+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -6.2692749694708
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0061000e+01 -3.1777000e-01 -1.4872000e-01 /
CHEB / 1.4272000e+00 3.9832000e-01 1.7772000e-01 /
CHEB / 5.0517000e-02 -3.7363000e-02 -4.3122000e-03 /
CHEB / 3.2893000e-02 -4.9564000e-02 -2.4846000e-02 /
CHEB / 3.7275000e-02 -4.6761000e-03 -5.6398000e-03 /

C4H6-13+H(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -22.057378842263603
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3885000e+00 -5.9538000e-01 -1.6054000e-01 /
CHEB / 3.7433000e+00 1.8329000e+00 -1.2515000e-02 /
CHEB / -1.3963000e+00 6.7092000e-01 1.1352000e-01 /
CHEB / -1.0399000e+00 6.0752000e-02 5.7313000e-02 /
CHEB / -5.8209000e-01 -1.0490000e-01 -7.2780000e-03 /

C4H6-13+H(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
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Cd/H2_Cd/H/De     H_rad       deltaHrxn(T=298K) = -46.26486491891474
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2292000e+01 4.7026000e-01 -3.9794000e-02 /
CHEB / -1.4242000e+00 7.9279000e-01 -4.5819000e-02 /
CHEB / -1.3349000e+00 4.8833000e-01 1.2764000e-03 /
CHEB / -8.9046000e-01 2.0259000e-01 2.3524000e-02 /
CHEB / -5.3363000e-01 2.1011000e-02 2.1718000e-02 /

C4H6-13+H(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -24.257154419815265
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3992000e+00 -3.4014000e-01 -1.9705000e-01 /
CHEB / 3.2473000e+00 1.8546000e+00 2.8574000e-02 /
CHEB / -1.4403000e+00 5.6952000e-01 9.6890000e-02 /
CHEB / -9.3404000e-01 2.4044000e-02 3.8836000e-02 /
CHEB / -4.8523000e-01 -8.4878000e-02 -3.7961000e-03 /

C4H6-13+H(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/De_Cd/H2     H_rad       deltaHrxn(T=298K) = -32.1562801442097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0696000e+01 2.0910000e-01 6.6404000e-02 /
CHEB / -9.1583000e-01 1.1396000e+00 -2.0411000e-01 /
CHEB / -1.7944000e+00 5.7284000e-01 2.3786000e-02 /
CHEB / -1.1551000e+00 1.5306000e-01 7.3232000e-02 /
CHEB / -6.2817000e-01 -6.8381000e-02 3.2121000e-02 /

C4H6-13+H(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -27.366894478300942
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3069000e+00 -9.4681000e-02 -2.2543000e-01 /
CHEB / 2.5026000e+00 1.5703000e+00 1.2176000e-01 /
CHEB / -1.4852000e+00 4.4258000e-01 5.7038000e-02 /
CHEB / -8.8235000e-01 5.0180000e-02 6.0306000e-03 /
CHEB / -4.4279000e-01 -3.4382000e-02 -5.9364000e-05 /

C4H6-13+H(+m)=aC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = 1.3098204830153222
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6490000e+00 -1.7417000e+00 -2.3613000e-01 /
CHEB / 6.2484000e+00 1.8091000e+00 1.4288000e-01 /
CHEB / -3.8418000e-02 1.9727000e-01 1.2762000e-01 /
CHEB / -1.5216000e-01 -1.5018000e-01 1.5804000e-02 /
CHEB / -4.1164000e-02 -1.0081000e-01 -2.4145000e-02 /
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C4H6-13+H(+m)=pC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = 0.35984177619602065
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2813000e+00 -1.4663000e+00 -2.3102000e-01 /
CHEB / 5.7938000e+00 1.5566000e+00 1.7306000e-01 /
CHEB / 1.9031000e-02 1.2005000e-01 8.7011000e-02 /
CHEB / -8.7368000e-02 -1.1923000e-01 9.9531000e-03 /
CHEB / -1.6013000e-02 -8.1538000e-02 -1.7469000e-02 /

aC3H4+CH3(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -23.367199325278918
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9395000e+00 6.0677000e-01 -2.5916000e-01 /
CHEB / 4.5132000e+00 1.7496000e+00 4.7519000e-02 /
CHEB / -1.5925000e+00 3.9466000e-01 1.4446000e-01 /
CHEB / -1.0516000e+00 3.7397000e-02 2.4298000e-02 /
CHEB / -5.5330000e-01 -9.7051000e-02 -2.2948000e-03 /

aC3H4+CH3(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -47.574685401930054
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5237000e+00 -2.6668000e-02 -3.3325000e-01 /
CHEB / 2.9665000e+00 2.3766000e+00 -4.4917000e-02 /
CHEB / -1.4688000e+00 7.2102000e-01 1.1803000e-01 /
CHEB / -1.0238000e+00 9.2164000e-02 3.8039000e-02 /
CHEB / -5.7679000e-01 -5.7909000e-02 -6.6517000e-03 /

aC3H4+CH3(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Ca     C_methyl         deltaHrxn(T=298K) = -25.56697490283058
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4884000e+00 8.9400000e-01 -1.2343000e-01 /
CHEB / 3.9947000e-01 8.9783000e-01 6.2595000e-02 /
CHEB / -1.7424000e+00 2.8479000e-01 6.7008000e-02 /
CHEB / -9.3510000e-01 -6.2972000e-03 2.1215000e-02 /
CHEB / -4.6106000e-01 -6.6140000e-02 -8.4989000e-03 /

aC3H4+CH3(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -33.46610062722502
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3034000e+00 5.6819000e-01 -3.8747000e-01 /
CHEB / 1.9521000e+00 2.0556000e+00 1.1042000e-01 /
CHEB / -1.8979000e+00 5.3249000e-01 5.5937000e-02 /
CHEB / -1.2142000e+00 2.3197000e-02 -4.3425000e-03 /
CHEB / -6.2961000e-01 -7.4225000e-02 -1.0479000e-02 /
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aC3H4+CH3(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -28.676714961316257
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8169000e-01 -2.0370000e-01 -3.5747000e-01 /
CHEB / 4.2776000e+00 2.5429000e+00 1.2622000e-01 /
CHEB / -1.1835000e+00 5.3494000e-01 9.8937000e-02 /
CHEB / -8.5114000e-01 2.8744000e-02 3.4255000e-02 /
CHEB / -4.6019000e-01 -6.4690000e-02 -1.6971000e-03 /

aC3H4+CH3(+m)=pC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -0.9499787068192944
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6354000e+00 -1.7073000e+00 -3.2221000e-01 /
CHEB / 7.6731000e+00 1.9217000e+00 2.6594000e-01 /
CHEB / 4.5461000e-01 1.9924000e-02 1.1177000e-01 /
CHEB / 3.7973000e-02 -1.6643000e-01 -5.4889000e-03 /
CHEB / 1.3300000e-02 -7.9175000e-02 -3.5271000e-02 /

C2H3+C2H4(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -26.757278539345748
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9069000e+00 -2.3653000e-01 -1.9715000e-01 /
CHEB / 2.2825000e+00 2.0202000e+00 4.7400000e-03 /
CHEB / -1.4253000e+00 6.9718000e-01 1.0520000e-01 /
CHEB / -1.0982000e+00 7.9612000e-02 5.5887000e-02 /
CHEB / -6.1140000e-01 -8.8032000e-02 -4.1219000e-04 /

C2H3+C2H4(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -50.964764615996884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8506000e+00 7.5537000e-03 -3.2621000e-01 /
CHEB / 9.0074000e-02 2.2196000e+00 -1.4516000e-02 /
CHEB / -1.7096000e+00 7.5570000e-01 1.1106000e-01 /
CHEB / -1.1103000e+00 1.0899000e-01 3.9333000e-02 /
CHEB / -6.1513000e-01 -5.8766000e-02 -7.5658000e-03 /

C2H3+C2H4(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -28.95705411689741
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1635000e+00 3.7440000e-01 -2.9056000e-01 /
CHEB / 1.2739000e+00 1.9918000e+00 1.3051000e-01 /
CHEB / -1.4801000e+00 4.4811000e-01 8.6219000e-02 /
CHEB / -9.6503000e-01 -4.1348000e-03 4.8443000e-03 /
CHEB / -4.9412000e-01 -5.9576000e-02 -9.9459000e-03 /

C2H3+C2H4(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
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Cd_pri_rad     Cd/H2_Cd/H2          deltaHrxn(T=298K) = -
36.85617984129185 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0960000e+00 1.2000000e+00 -2.1401000e-01 /
CHEB / -1.4417000e+00 1.2646000e+00 -1.6167000e-02 /
CHEB / -2.1539000e+00 5.1149000e-01 1.5857000e-02 /
CHEB / -1.2474000e+00 1.0561000e-01 6.5097000e-03 /
CHEB / -6.4880000e-01 -4.3492000e-02 5.3602000e-05 /

C2H3+C2H4(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -32.06679417538309
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7256000e+00 -4.0609000e-01 -3.9240000e-01 /
CHEB / 1.7985000e+00 2.6913000e+00 1.7972000e-01 /
CHEB / -1.4854000e+00 5.4910000e-01 1.1776000e-01 /
CHEB / -9.7018000e-01 8.3176000e-03 2.0664000e-02 /
CHEB / -4.9692000e-01 -6.5774000e-02 -8.1126000e-03 /

C2H3+C2H4(+m)=C4H6-13+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -4.699899697082152
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0470000e+00 -1.2888000e+00 -6.4712000e-02 /
CHEB / 3.0653000e+00 1.1888000e+00 -5.1166000e-02 /
CHEB / 2.5056000e-02 3.1976000e-01 1.0842000e-01 /
CHEB / -1.1284000e-01 -7.8151000e-02 5.7617000e-02 /
CHEB / -4.6152000e-02 -1.0926000e-01 -1.2928000e-02 /

C2H3+C2H4(+m)=aC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -3.390079214066823
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9227000e+00 -1.2947000e+00 -2.8138000e-01 /
CHEB / 4.8102000e+00 1.4793000e+00 2.5777000e-01 /
CHEB / 2.0705000e-01 -7.4113000e-03 7.7848000e-02 /
CHEB / -4.0280000e-02 -1.3882000e-01 -2.6965000e-02 /
CHEB / -4.4632000e-03 -4.9943000e-02 -2.2450000e-02 /

C2H3+C2H4(+m)=pC3H4+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -4.3400579208861245
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3588000e+00 -1.9068000e+00 -3.6124000e-01 /
CHEB / 5.3375000e+00 2.1340000e+00 2.9549000e-01 /
CHEB / 1.7288000e-01 4.0449000e-02 1.3135000e-01 /
CHEB / -6.6800000e-02 -1.8915000e-01 -1.0482000e-02 /
CHEB / -1.2836000e-02 -9.0925000e-02 -3.9316000e-02 /

pC3H4+CH3(+m)=C4H7-11(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -22.417220618459623
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3337000e-01 -4.9454000e-01 -3.0718000e-01 /
CHEB / 5.1603000e+00 2.4493000e+00 1.3551000e-01 /
CHEB / -1.2028000e+00 5.5702000e-01 1.1443000e-01 /
CHEB / -9.8244000e-01 1.7151000e-02 3.6863000e-02 /
CHEB / -5.4989000e-01 -9.6453000e-02 -1.3927000e-02 /

pC3H4+CH3(+m)=C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -46.62470669511076
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0110000e+00 4.7112000e-01 -3.1170000e-01 /
CHEB / 2.5902000e+00 1.9215000e+00 4.8974000e-02 /
CHEB / -1.4795000e+00 5.3392000e-01 2.5816000e-02 /
CHEB / -9.5662000e-01 1.1339000e-01 4.4947000e-03 /
CHEB / -5.2827000e-01 -9.4900000e-03 7.4007000e-03 /

pC3H4+CH3(+m)=C4H7-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -24.616996196011286
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3984000e-01 -1.6416000e-01 -3.5106000e-01 /
CHEB / 4.7400000e+00 2.5256000e+00 1.4077000e-01 /
CHEB / -1.1618000e+00 4.8859000e-01 1.1227000e-01 /
CHEB / -8.4747000e-01 -1.1246000e-02 3.5326000e-02 /
CHEB / -4.5743000e-01 -8.6749000e-02 -8.0693000e-03 /

pC3H4+CH3(+m)=C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -32.51612192040572
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6571000e+00 -2.2655000e-01 -4.7877000e-01 /
CHEB / 2.7906000e+00 2.8286000e+00 1.4891000e-01 /
CHEB / -1.8738000e+00 5.6744000e-01 1.2976000e-01 /
CHEB / -1.2122000e+00 -1.8163000e-02 1.7338000e-02 /
CHEB / -6.2876000e-01 -1.0423000e-01 -2.0330000e-02 /

pC3H4+CH3(+m)=C4H7-22(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond exact:
Ct/H_Ct/Nd     C_methyl       deltaHrxn(T=298K) = -27.726736254496963
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7029000e+00 1.1448000e+00 -1.6655000e-01 /
CHEB / 3.9248000e-01 7.6935000e-01 1.2433000e-01 /
CHEB / -1.8448000e+00 1.7381000e-01 5.3809000e-02 /
CHEB / -9.2758000e-01 -2.3508000e-02 1.0602000e-03 /
CHEB / -4.3250000e-01 -4.1724000e-02 -1.1125000e-02 /

C4H6-2+H(+m)=C4H7-11(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -27.806745449793254
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 2.6070000e+00 -6.0219000e-01 -2.9434000e-01 /
CHEB / 3.4672000e+00 2.4273000e+00 1.3593000e-01 /
CHEB / -1.2210000e+00 5.5433000e-01 1.0867000e-01 /
CHEB / -1.0255000e+00 1.8608000e-02 3.7134000e-02 /
CHEB / -5.8246000e-01 -9.5058000e-02 -1.2052000e-02 /

C4H6-2+H(+m)=C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -52.01423152644439
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0280000e+00 3.1425000e-01 -2.9060000e-01 /
CHEB / 8.5538000e-01 1.8671000e+00 6.1827000e-02 /
CHEB / -1.5172000e+00 5.4140000e-01 2.4973000e-02 /
CHEB / -1.0022000e+00 1.0983000e-01 2.1548000e-03 /
CHEB / -5.5969000e-01 -1.1120000e-02 6.6734000e-03 /

C4H6-2+H(+m)=C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -30.006521027344917
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2781000e+00 -3.4257000e-01 -3.2068000e-01 /
CHEB / 3.0564000e+00 2.5219000e+00 1.3180000e-01 /
CHEB / -1.1964000e+00 4.9844000e-01 1.0835000e-01 /
CHEB / -8.9693000e-01 -1.0519000e-02 3.5447000e-02 /
CHEB / -4.9115000e-01 -8.7319000e-02 -7.2784000e-03 /

C4H6-2+H(+m)=C4H7-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -37.905646751739354
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6518000e+00 -4.0601000e-01 -4.5520000e-01 /
CHEB / 1.0745000e+00 2.7909000e+00 1.5761000e-01 /
CHEB / -1.9055000e+00 5.8140000e-01 1.2763000e-01 /
CHEB / -1.2588000e+00 -2.0663000e-02 1.7246000e-02 /
CHEB / -6.6100000e-01 -1.0624000e-01 -1.9610000e-02 /

C4H6-2+H(+m)=C4H7-22(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Ct/Nd_Ct/Nd     H_rad          deltaHrxn(T=298K) = -
33.116261085830594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0237000e+01 6.9057000e-01 -5.4979000e-03 /
CHEB / -1.6183000e+00 8.0045000e-01 5.7672000e-02 /
CHEB / -1.8393000e+00 2.1024000e-01 4.4856000e-02 /
CHEB / -9.7547000e-01 -1.4187000e-02 3.5144000e-03 /
CHEB / -4.6850000e-01 -4.2409000e-02 -1.0940000e-02 /

C4H6-2+H(+m)=C2H2+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -1.2697357738110462
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 2.3160000e+00 -2.1045000e+00 -3.1220000e-01 /
CHEB / 6.3719000e+00 2.2065000e+00 2.0369000e-01 /
CHEB / 9.7191000e-02 2.1542000e-01 1.5742000e-01 /
CHEB / -2.2902000e-01 -1.7477000e-01 1.9830000e-02 /
CHEB / -1.0025000e-01 -1.3295000e-01 -4.0047000e-02 /

C4H6-2+H(+m)=C4H6-13+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -5.749366607529659
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8648000e+00 -1.5535000e+00 -2.2286000e-01 /
CHEB / 4.2139000e+00 1.6175000e+00 1.6464000e-01 /
CHEB / 1.6000000e-01 1.5944000e-01 8.1400000e-02 /
CHEB / -6.1648000e-02 -1.1850000e-01 1.2822000e-02 /
CHEB / -2.6285000e-02 -8.7686000e-02 -1.3012000e-02 /

C4H6-2+H(+m)=aC3H4+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -4.4395461245143295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1153000e+00 -1.7862000e+00 -3.1462000e-01 /
CHEB / 6.2338000e+00 1.9923000e+00 2.5132000e-01 /
CHEB / 3.8743000e-01 4.0363000e-02 1.1523000e-01 /
CHEB / -2.2552000e-02 -1.6917000e-01 -2.9273000e-04 /
CHEB / -2.3880000e-02 -8.5315000e-02 -3.3983000e-02 /

C4H6-2+H(+m)=C2H3+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -1.0494669104475118
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8258000e+00 -1.9925000e+00 -3.5377000e-01 /
CHEB / 4.8320000e+00 2.2106000e+00 2.8158000e-01 /
CHEB / 4.7262000e-02 6.2768000e-02 1.3367000e-01 /
CHEB / -1.3053000e-01 -1.9249000e-01 -5.0061000e-03 /
CHEB / -4.8389000e-02 -9.6916000e-02 -3.7691000e-02 /

C4H6-2+H(+m)=pC3H4+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7-11)      deltaHrxn(T=298K) = -5.389524831333631
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1475000e+01 -5.6520000e-01 -1.4246000e-01 /
CHEB / 2.1018000e+00 6.9090000e-01 1.5187000e-01 /
CHEB / -1.5720000e-01 -4.3948000e-02 2.1178000e-02 /
CHEB / -6.9662000e-02 -8.5396000e-02 -2.3969000e-02 /
CHEB / -1.0137000e-02 -1.4868000e-02 -1.1694000e-02 /

!PDepNetwork iC4H7 + HCC[CH3]2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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```
!     iC4H7             35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62
      50.57
!     HCC[CH3]2         55.3  72.75 21.39 25.9  29.94 33.42 39.09 43.4
      50.18 null
!     C4H7J(142)        49.97 70.87 17.72 22.41 26.98 31.04 37.53 42.37
      50.1  null
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     pC3H4             46.16 58.99 14.37 17.14 19.55 21.6  24.93 27.49
      31.65
!Here are the path reactions and their high-P limit kinetics:
!     aC3H4+CH3=iC4H7         1.5800000e+11      0.00000
4.9700000e+03
!     HCC[CH3]2=iC4H7               1.8360000e+11      0.97000
3.7700000e+04
!     pC3H4+CH3=HCC[CH3]2     1.9900000e+13      0.00000
1.2100000e+04

HCC[CH3]2(+m)=iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#61 (iC4H7) High-P Limit: intra_H_migration exact:  R3H_DS
Cd_rad_out_singleH     Cs_H_out_2H        deltaHrxn(T=298K) = -
20.09765691088011 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4196000e+00 8.8491000e-01 -9.2221000e-02 /
CHEB / 1.0055000e+01 1.0400000e+00 9.9747000e-03 /
CHEB / -1.9211000e+00 3.2397000e-01 5.7754000e-02 /
CHEB / -1.1161000e+00 -3.4879000e-03 2.3639000e-02 /
CHEB / -5.8393000e-01 -7.9848000e-02 -2.7988000e-03 /

aC3H4+CH3(+m)=iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#61 (iC4H7) High-P Limit: R_Addition_MultipleBond exact:  Ca_Cd/H2
C_methyl          deltaHrxn(T=298K) = -47.15466058166173 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3460000e+00 4.4401000e-01 -4.0437000e-02 /
CHEB / 2.4363000e-01 7.4369000e-01 -4.3107000e-02 /
CHEB / -1.1286000e+00 4.4221000e-01 1.4824000e-02 /
CHEB / -7.1981000e-01 1.6885000e-01 3.9889000e-02 /
CHEB / -4.3481000e-01 1.1922000e-02 2.9421000e-02 /

aC3H4+CH3(+m)=HCC[CH3]2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #61 (iC4H7) deltaHrxn(T=298K) = -27.05700367078162 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9036000e+00 -4.2818000e-01 -1.2657000e-01 /
CHEB / 2.7103000e+00 1.7152000e+00 4.0365000e-02 /
CHEB / -1.2793000e+00 4.6389000e-01 7.8249000e-02 /
CHEB / -8.5580000e-01 2.3019000e-02 2.2733000e-02 /
CHEB / -4.5746000e-01 -5.2684000e-02 4.3547000e-04 /

!aC3H4+CH3(+m)=pC3H4+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #61 (iC4H7) deltaHrxn(T=298K) = -0.9499787068192944 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
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```
!CHEB / 5.2957000e+00 -1.6299000e+00 -2.3662000e-01 /
!CHEB / 5.9246000e+00 1.6524000e+00 1.5444000e-01 /
!CHEB / -1.1693000e-02 1.8420000e-01 9.9185000e-02 /
!CHEB / -1.7271000e-01 -9.4492000e-02 1.9969000e-02 /
!CHEB / -8.3587000e-02 -7.9264000e-02 -1.0332000e-02 /

pC3H4+CH3(+m)=iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#61 (iC4H7) deltaHrxn(T=298K) = -46.204681874842436 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0780000e+00 2.4184000e-02 -2.5331000e-01 /
CHEB / 3.7488000e+00 1.7768000e+00 7.7507000e-02 /
CHEB / -1.1869000e+00 4.7647000e-01 8.2571000e-02 /
CHEB / -8.1025000e-01 5.7125000e-02 3.3193000e-02 /
CHEB / -4.5141000e-01 -2.9818000e-02 1.1101000e-02 /

pC3H4+CH3(+m)=HCC[CH3]2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #61 (iC4H7) High-P Limit: R_Addition_MultipleBond exact:
Ct/Nd_Ct/H     C_methyl       deltaHrxn(T=298K) = -26.107024963962324
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5425000e+00 9.6230000e-01 -1.2847000e-01 /
CHEB / 1.2083000e+00 9.1171000e-01 6.7093000e-02 /
CHEB / -1.7718000e+00 2.8119000e-01 5.2409000e-02 /
CHEB / -9.2631000e-01 4.4322000e-03 1.1187000e-02 /
CHEB / -4.4933000e-01 -4.6201000e-02 -9.7544000e-03 /

!PDepNetwork C3H6O && C3H6O-enol
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H6O             -44.5 72.73 19.42 23.41 26.92 29.97 35.32 39.17
      43.85 Estimated by Group Additivity
!     C3H6O-enol        -37.48      71.5  19.4  23.83 27.67 30.87 35.79
      39.39 45.1  Estimated by Group Additivity
!     CH3               35.1  46.36 9.2   9.98  10.75 11.5  12.86 14.08
      16.29 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009089)
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 Estimated by Group Additivity
!     C3H5O-enol2             -1.38 69.74 18.78 23.27 26.89 29.75 33.95
      36.93 41.61 Estimated by Group Additivity
!     H           52.1  27.41 4.97  4.97  4.97  4.97  4.97  4.97  4.97
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009800)
!     C3H5OJ(17)        19.42 73.31 19.06 22.62 25.73 28.35 32.45 35.48
      40.34 Estimated by Group Additivity
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 Estimated by Group Additivity
!     OH          9.4   43.91 7.14  7.07  7.05  7.06  7.15  7.34  7.87
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00010102)
!     CH3CHcOH          21.62 72.89 19.21 23.08 26.31 28.95 32.97 35.9
      40.57 Estimated by Group Additivity
!     C3H5OJ(12)        -1.58 70.39 18.06 21.84 25.19 28.08 32.66 36.06
      41.31 Estimated by Group Additivity
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!     CH2CHO            6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34
      26.35 Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002559)
!     C3H5OJ(13)        4.5   76.14 18.65 22.05 25.01 27.57 32.16 35.43
      39.19 Estimated by Group Additivity
!     C2H5        28.36 59.05 12.11 14.59 17.07 19.35 22.93 25.78 30.3
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00002703)
!     HCO         10.04 53.61 8.27  8.72  9.24  9.78  10.74 11.49 12.59
      Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009325)
!     C3H5OJ(8)         -7.6  73.85 18.59 21.98 24.96 27.55 32.16 35.44
      39.21 Estimated by Group Additivity
!     C2H6              -20.04      54.77 12.6  15.57 18.58 21.36 25.8
      29.32 34.88 Primary Thermo Library: GRI-Mech3.0 (Species ID:
s00002784)
!     CO          -26.42      47.23 6.96  7.02  7.12  7.27  7.62  7.93
      8.41  Primary Thermo Library: GRI-Mech3.0 (Species ID: s00009358)
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol=C3H6O              8.590e+11    0.32        55900.00
!     CH3+C2H3O-1=C3H6O-enol  7.230e+13    0.00        0.00
!     C3H5O-enol2+H=C3H6O-enol      5.000e+13    0.00        0.00
!     C3H5OJ(17)+H=C3H6O-enol       1.000e+13    0.00        0.00
!     pC3H5+OH=C3H6O-enol     1.000e+13    0.00        0.00
!     CH3CHcOH+H=C3H6O-enol   1.000e+13    0.00        0.00
!     C3H5OJ(12)+H=C3H6O-enol       1.000e+13    0.00        0.00
!     CH3+CH2CHO=C3H6O        1.000e+13    0.00        0.00
!     C3H5OJ(13)+H=C3H6O            1.000e+14    0.00        0.00
!     C2H5+HCO=C3H6O          1.810e+13    0.00        0.00
!     C3H5OJ(12)+H=C3H6O            5.000e+13    0.00        0.00
!     C3H5OJ(8)+H=C3H6O       1.000e+13    0.00        0.00
!     C2H6+CO=C3H6O           9.140e+04    2.53        85500.00

C3H6O-enol(+m)=C3H6O(+m)                          1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
ReactionLibrary: Tautomerization    deltaHrxn(T=298K) = -
7.019396965630307 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.0641000e+01 2.2346000e-01 -3.8261000e-02 1.4963000e-03 /
CHEB / 1.6844000e+01 4.1164000e-01 -6.5735000e-02 9.8718000e-04 /
CHEB / -3.4008000e-01 3.2106000e-01 -3.9667000e-02 -3.2297000e-03 /
CHEB / -2.6067000e-01 2.1041000e-01 -1.1910000e-02 -6.1892000e-03 /

CH3+C2H3O-1(+m)=C3H6O(+m)                         1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
109.08336468329485 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0887000e+01 1.8150000e+00 -1.0703000e+00 1.8503000e-01 /
CHEB / -1.5068000e+00 2.2611000e+00 -1.0856000e-01 -1.9001000e-01 /
CHEB / -8.3559000e-01 6.9395000e-01 1.7886000e-01 -1.1104000e-01 /
CHEB / -3.8618000e-01 1.6380000e-01 1.1650000e-01 -1.9339000e-02 /

CH3+C2H3O-1(+m)=C3H6O-enol(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination exact:  [ C_methyl , Cd_pri_rad ]     deltaHrxn(T=298K)
= -102.06396771766454 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
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CHEB / 1.1691000e+01 2.9523000e+00 -1.0374000e+00 2.0192000e-01 /
CHEB / -2.2215000e+00 2.0878000e+00 -1.0050000e-01 -2.5014000e-01 /
CHEB / -9.9214000e-01 6.1810000e-01 2.1947000e-01 -1.3372000e-01 /
CHEB / -4.2462000e-01 1.3498000e-01 1.4625000e-01 -1.9824000e-02 /

C3H5O-enol2+H(+m)=C3H6O(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
95.2063950869945 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1748000e+01 -3.0268000e-01 -4.3243000e-01 7.7150000e-02 /
CHEB / -4.1232000e-01 1.8337000e+00 -1.7409000e-01 -5.8561000e-02 /
CHEB / -5.4305000e-01 7.4602000e-01 6.1614000e-02 -5.7330000e-02 /
CHEB / -3.3853000e-01 2.1629000e-01 7.7561000e-02 -1.9360000e-02 /

C3H5O-enol2+H(+m)=C3H6O-enol(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/Cd , H_rad ]
      deltaHrxn(T=298K) = -88.1869981213642 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2809000e+01 1.1618000e+00 -3.4684000e-01 6.3299000e-02 /
CHEB / -1.3583000e+00 1.3747000e+00 -1.8741000e-01 -7.0614000e-02 /
CHEB / -7.4295000e-01 5.9926000e-01 6.3847000e-02 -8.4631000e-02 /
CHEB / -3.6358000e-01 1.9949000e-01 9.6222000e-02 -3.1963000e-02 /

C3H5O-enol2+H(+m)=CH3+C2H3O-1(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) =
13.876969596300338 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.7300000e+00 -9.2523000e-01 -2.2171000e-01 2.0900000e-02 /
CHEB / 5.6123000e+00 8.0543000e-01 9.7181000e-02 -6.2739000e-02 /
CHEB / 1.8499000e-01 1.8508000e-01 1.1095000e-01 9.0258000e-03 /
CHEB / -5.1240000e-02 -1.4978000e-02 3.3588000e-02 2.5070000e-02 /

C3H5OJ(17)+H(+m)=C3H6O(+m)                      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
116.00420851526499 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.1957000e+00 2.9211000e+00 -1.3672000e+00 2.0467000e-01 /
CHEB / -1.8384000e+00 2.3716000e+00 1.2266000e-02 -3.1108000e-01 /
CHEB / -9.2166000e-01 6.2936000e-01 2.5933000e-01 -1.2693000e-01 /
CHEB / -4.1408000e-01 1.2618000e-01 1.3879000e-01 -1.4321000e-02 /

C3H5OJ(17)+H(+m)=C3H6O-enol(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ Cd_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -108.98481154963468 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9636000e+00 3.9969000e+00 -1.3716000e+00 2.0769000e-01 /
CHEB / -2.5166000e+00 2.2603000e+00 5.6558000e-02 -3.5963000e-01 /
CHEB / -1.0741000e+00 5.6124000e-01 3.0628000e-01 -1.4518000e-01 /
CHEB / -4.5625000e-01 9.1187000e-02 1.6539000e-01 -1.5229000e-02 /
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C3H5OJ(17)+H(+m)=CH3+C2H3O-1(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -6.920843831970149
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1113000e+01 -7.9716000e-01 -2.2065000e-01 9.9243000e-03 /
CHEB / 1.6105000e+00 7.6665000e-01 1.3959000e-01 -4.9785000e-02 /
CHEB / 2.7994000e-01 1.1886000e-01 9.9054000e-02 2.2843000e-02 /
CHEB / -3.1693000e-02 -4.3246000e-02 9.7521000e-03 2.1644000e-02 /

C3H5OJ(17)+H(+m)=C3H5O-enol2+H(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
20.797813428270487 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0279000e+01 -8.0543000e-01 -2.3643000e-01 9.4268000e-03 /
CHEB / 1.2213000e+00 7.2766000e-01 1.3990000e-01 -5.2637000e-02 /
CHEB / 2.2394000e-01 1.4934000e-01 1.0139000e-01 1.9857000e-02 /
CHEB / -1.5027000e-02 -2.2816000e-02 1.9671000e-02 2.2907000e-02 /

pC3H5+OH(+m)=C3H6O(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -117.63987722151019
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.8959000e+00 3.3382000e+00 -1.4745000e+00 2.0143000e-01 /
CHEB / -1.9726000e+00 2.3976000e+00 7.2225000e-02 -3.5155000e-01 /
CHEB / -9.4910000e-01 5.9832000e-01 2.9042000e-01 -1.2914000e-01 /
CHEB / -4.2118000e-01 1.0906000e-01 1.4659000e-01 -1.2614000e-02 /

pC3H5+OH(+m)=C3H6O-enol(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O) High-P Limit: R_Recombination estimate:
(Average:) [ Cd_pri_rad , O_pri_rad ]     deltaHrxn(T=298K) = -
110.62048025587988 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.6573000e+00 4.4021000e+00 -1.4878000e+00 1.9911000e-01 /
CHEB / -2.6440000e+00 2.2988000e+00 1.2575000e-01 -3.9458000e-01 /
CHEB / -1.1010000e+00 5.3127000e-01 3.3826000e-01 -1.4677000e-01 /
CHEB / -4.6417000e-01 7.2618000e-02 1.7215000e-01 -1.4100000e-02 /

pC3H5+OH(+m)=CH3+C2H3O-1(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -8.556512538215348
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1388000e+01 -7.6168000e-01 -2.2328000e-01 6.2886000e-03 /
CHEB / 1.3698000e+00 7.4011000e-01 1.5090000e-01 -4.5552000e-02 /
CHEB / 2.5201000e-01 1.0958000e-01 9.3780000e-02 2.5002000e-02 /
CHEB / -2.7888000e-02 -4.5045000e-02 5.8599000e-03 2.0166000e-02 /

pC3H5+OH(+m)=C3H5O-enol2+H(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -22.433482134515685
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0428000e+01 -7.6103000e-01 -2.3891000e-01 3.9911000e-03 /
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CHEB / 1.0921000e+00 6.9840000e-01 1.5303000e-01 -4.6709000e-02 /
CHEB / 1.9205000e-01 1.3562000e-01 9.6594000e-02 2.3019000e-02 /
CHEB / -1.8224000e-02 -2.5917000e-02 1.4599000e-02 2.1618000e-02 /

C3H5OJ(17)+H(+m)=pC3H5+OH(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = 1.6356687062452018
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.7929000e+00 -7.3639000e-01 -2.1749000e-01 4.1817000e-03 /
CHEB / 2.7130000e+00 7.4123000e-01 1.5594000e-01 -4.2006000e-02 /
CHEB / 3.0809000e-01 8.5149000e-02 8.9147000e-02 2.7610000e-02 /
CHEB / -2.1930000e-02 -5.2266000e-02 -1.0549000e-03 1.8195000e-02 /

CH3CHcOH+H(+m)=C3H6O(+m)                        1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
118.20398400189757 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.0433000e+00 3.2538000e+00 -1.4531000e+00 2.0259000e-01 /
CHEB / -2.0092000e+00 2.3930000e+00 5.9573000e-02 -3.4381000e-01 /
CHEB / -9.4384000e-01 6.0486000e-01 2.8417000e-01 -1.2884000e-01 /
CHEB / -4.1827000e-01 1.1263000e-01 1.4506000e-01 -1.2936000e-02 /

CH3CHcOH+H(+m)=C3H6O-enol(+m)                   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ Cd_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -111.18458703626726 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.8058000e+00 4.3198000e+00 -1.4648000e+00 2.0126000e-01 /
CHEB / -2.6817000e+00 2.2921000e+00 1.1146000e-01 -3.8788000e-01 /
CHEB / -1.0958000e+00 5.3764000e-01 3.3187000e-01 -1.4657000e-01 /
CHEB / -4.6112000e-01 7.6437000e-02 1.7081000e-01 -1.4306000e-02 /

CH3CHcOH+H(+m)=CH3+C2H3O-1(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -9.120619318602724
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1421000e+01 -7.6905000e-01 -2.2280000e-01 7.0798000e-03 /
CHEB / 1.3526000e+00 7.4568000e-01 1.4866000e-01 -4.6491000e-02 /
CHEB / 2.5772000e-01 1.1152000e-01 9.4891000e-02 2.4586000e-02 /
CHEB / -2.7092000e-02 -4.4718000e-02 6.6492000e-03 2.0483000e-02 /

CH3CHcOH+H(+m)=C3H5O-enol2+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
22.997588914903062 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0485000e+01 -7.6999000e-01 -2.3854000e-01 5.1217000e-03 /
CHEB / 1.0542000e+00 7.0434000e-01 1.5050000e-01 -4.7979000e-02 /
CHEB / 1.9819000e-01 1.3841000e-01 9.7620000e-02 2.2418000e-02 /
CHEB / -1.6095000e-02 -2.5294000e-02 1.5614000e-02 2.1898000e-02 /
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CH3CHcOH+H(+m)=C3H5OJ(17)+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -2.199775486632582
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.8014000e+00 -7.4173000e-01 -2.1737000e-01 4.7187000e-03 /
CHEB / 2.4211000e+00 7.4507000e-01 1.5440000e-01 -4.2708000e-02 /
CHEB / 4.0235000e-01 8.6789000e-02 9.0130000e-02 2.7336000e-02 /
CHEB / 4.7394000e-03 -5.1894000e-02 -4.5473000e-04 1.8482000e-02 /

CH3CHcOH+H(+m)=pC3H5+OH(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -0.5641067803873732
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.2092000e+00 -7.2239000e-01 -2.1658000e-01 2.8014000e-03 /
CHEB / 2.3300000e+00 7.3440000e-01 1.5927000e-01 -4.0061000e-02 /
CHEB / 3.1584000e-01 7.7516000e-02 8.6557000e-02 2.8495000e-02 /
CHEB / -1.7961000e-02 -5.3662000e-02 -3.3276000e-03 1.7274000e-02 /

C3H5OJ(12)+H(+m)=C3H6O(+m)                      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H/OneDeC , H_rad ]
      deltaHrxn(T=298K) = -95.0064655055115 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2742000e+01 1.0857000e+00 -2.9501000e-01 5.2260000e-02 /
CHEB / -1.3213000e+00 8.7684000e-01 -3.5328000e-02 -2.8433000e-02 /
CHEB / -7.2225000e-01 3.8016000e-01 1.5374000e-02 -8.5285000e-03 /
CHEB / -3.5602000e-01 1.1926000e-01 2.1059000e-02 -7.6905000e-03 /

C3H5OJ(12)+H(+m)=C3H6O-enol(+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ O_rad/OneDe , H_rad ]
      deltaHrxn(T=298K) = -87.9870685398812 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2280000e+01 1.0191000e+00 -3.0486000e-01 6.5459000e-02 /
CHEB / -1.2717000e+00 1.2196000e+00 -1.5176000e-01 -6.3013000e-02 /
CHEB / -6.8254000e-01 5.3941000e-01 6.7570000e-02 -7.2284000e-02 /
CHEB / -3.4585000e-01 1.8273000e-01 8.9090000e-02 -2.1182000e-02 /

C3H5OJ(12)+H(+m)=CH3+C2H3O-1(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = 14.07689917778335
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.0957000e+00 -9.2674000e-01 -2.2247000e-01 2.0842000e-02 /
CHEB / 5.5713000e+00 8.0609000e-01 9.7426000e-02 -6.2892000e-02 /
CHEB / 1.8697000e-01 1.8576000e-01 1.1129000e-01 9.0941000e-03 /
CHEB / -5.5654000e-02 -1.4863000e-02 3.3658000e-02 2.5116000e-02 /

C3H5OJ(12)+H(+m)=C3H5O-enol2+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) =
0.199929581483012 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
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CHEB / 8.1476000e+00 -1.1551000e+00 -1.6842000e-01 2.2395000e-02 /
CHEB / 3.1234000e+00 9.3298000e-01 -6.4895000e-03 -5.1086000e-02 /
CHEB / 4.9979000e-01 2.6353000e-01 1.1340000e-01 -1.8236000e-02 /
CHEB / -6.7528000e-03 2.8653000e-03 6.1641000e-02 2.0480000e-02 /

C3H5OJ(17)+H(+m)=C3H5OJ(12)+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
20.997743009753492 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7828000e+00 -8.0597000e-01 -2.3686000e-01 9.2810000e-03 /
CHEB / 9.8951000e-01 7.2784000e-01 1.4007000e-01 -5.2629000e-02 /
CHEB / 1.7295000e-01 1.4960000e-01 1.0158000e-01 1.9925000e-02 /
CHEB / -3.0101000e-02 -2.2727000e-02 1.9716000e-02 2.2928000e-02 /

pC3H5+OH(+m)=C3H5OJ(12)+H(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -22.63341171599869
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9313000e+00 -7.6137000e-01 -2.3924000e-01 3.8551000e-03 /
CHEB / 8.6014000e-01 6.9851000e-01 1.5316000e-01 -4.6689000e-02 /
CHEB / 1.4108000e-01 1.3580000e-01 9.6745000e-02 2.3080000e-02 /
CHEB / -3.3286000e-02 -2.5840000e-02 1.4640000e-02 2.1638000e-02 /

CH3CHcOH+H(+m)=C3H5OJ(12)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -23.197518496386067
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9885000e+00 -7.7037000e-01 -2.3888000e-01 4.9828000e-03 /
CHEB / 8.2226000e-01 7.0446000e-01 1.5064000e-01 -4.7960000e-02 /
CHEB / 1.4722000e-01 1.3860000e-01 9.7779000e-02 2.2480000e-02 /
CHEB / -3.1159000e-02 -2.5214000e-02 1.5656000e-02 2.1918000e-02 /

CH3+CH2CHO(+m)=C3H6O(+m)                  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O) High-P Limit: R_Recombination estimate:
(Average:) [ C_methyl , C_rad/H2/CO ]     deltaHrxn(T=298K) = -
85.59277991340406 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2531000e+01 4.7272000e-01 -8.0335000e-02 9.6058000e-03 /
CHEB / -9.6941000e-01 6.9773000e-01 -6.6029000e-02 -7.9012000e-03 /
CHEB / -6.0253000e-01 3.5544000e-01 1.1304000e-02 -1.1152000e-02 /
CHEB / -3.1619000e-01 1.3130000e-01 2.5770000e-02 -9.5815000e-04 /

CH3+CH2CHO(+m)=C3H6O-enol(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -78.57338294777375
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0308000e+01 -9.1250000e-01 -1.9988000e-01 2.5628000e-02 /
CHEB / 2.4538000e-01 1.5359000e+00 -1.5106000e-01 -2.4061000e-02 /
CHEB / -3.9401000e-01 7.0543000e-01 3.8237000e-02 -3.5902000e-02 /
CHEB / -3.1986000e-01 2.1588000e-01 6.4368000e-02 -1.1155000e-02 /
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CH3+C2H3O-1(+m)=CH3+CH2CHO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -23.49058476989078
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1969000e+01 -1.1557000e+00 -3.8201000e-01 -1.8002000e-02 /
CHEB / 7.2221000e-01 1.0196000e+00 2.4543000e-01 -3.6847000e-02 /
CHEB / 3.2512000e-02 2.0865000e-01 1.2528000e-01 1.7195000e-02 /
CHEB / -7.3522000e-02 -2.0439000e-02 2.6905000e-02 2.2835000e-02 /

C3H5O-enol2+H(+m)=CH3+CH2CHO(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -9.613615173590437
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0733000e+01 -1.9917000e+00 -3.3493000e-01 2.9512000e-02 /
CHEB / 1.8583000e+00 1.6909000e+00 9.4821000e-02 -7.7834000e-02 /
CHEB / 1.8868000e-01 3.6677000e-01 1.5463000e-01 -1.0122000e-02 /
CHEB / -9.2159000e-02 -3.0488000e-02 6.0934000e-02 1.7225000e-02 /

C3H5OJ(17)+H(+m)=CH3+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -30.411428601860926
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1252000e+01 -8.8648000e-01 -3.3946000e-01 -3.1398000e-02 /
CHEB / 4.9691000e-01 8.0228000e-01 2.3832000e-01 -2.0754000e-02 /
CHEB / -3.2799000e-02 1.5977000e-01 1.1081000e-01 2.6668000e-02 /
CHEB / -8.8576000e-02 -2.0109000e-02 1.6516000e-02 2.1730000e-02 /

pC3H5+OH(+m)=CH3+CH2CHO(+m)         1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -32.047097308106125 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1317000e+01 -8.0569000e-01 -3.2329000e-01 -3.4106000e-02 /
CHEB / 4.0541000e-01 7.3966000e-01 2.3482000e-01 -1.6748000e-02 /
CHEB / -5.5316000e-02 1.4305000e-01 1.0469000e-01 2.9740000e-02 /
CHEB / -9.1958000e-02 -2.1757000e-02 1.2436000e-02 2.1197000e-02 /

CH3CHcOH+H(+m)=CH3+CH2CHO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -32.6112040884935
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1391000e+01 -8.2130000e-01 -3.2649000e-01 -3.3592000e-02 /
CHEB / 3.6012000e-01 7.5164000e-01 2.3547000e-01 -1.7546000e-02 /
CHEB / -5.0991000e-02 1.4639000e-01 1.0598000e-01 2.9143000e-02 /
CHEB / -8.9778000e-02 -2.1364000e-02 1.3272000e-02 2.1322000e-02 /

C3H5OJ(12)+H(+m)=CH3+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -9.413685592107425
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1938000e+01 -8.4673000e-01 -1.8512000e-01 1.2521000e-02 /
CHEB / 9.1101000e-01 7.9311000e-01 1.1458000e-01 -3.8267000e-02 /
CHEB / 1.3991000e-01 1.3411000e-01 7.3815000e-02 1.3344000e-02 /
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CHEB / -2.8540000e-02 -4.4067000e-02 9.0602000e-03 1.0870000e-02 /

C3H5OJ(13)+H(+m)=C3H6O(+m)                      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination exact:  [ C_rad/H2/Cs , H_rad ] deltaHrxn(T=298K) = -
101.08568577022801 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2048000e+01 2.2811000e+00 -6.0570000e-01 3.1247000e-02 /
CHEB / -1.5236000e+00 7.3041000e-01 1.2352000e-01 7.2973000e-03 /
CHEB / -8.1185000e-01 3.0160000e-01 5.2054000e-02 7.3317000e-03 /
CHEB / -3.7159000e-01 7.7349000e-02 1.9780000e-02 -1.8043000e-03 /

C3H5OJ(13)+H(+m)=C3H6O-enol(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
94.0662888045977 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0683000e+01 9.8948000e-01 -8.0898000e-01 1.2029000e-01 /
CHEB / -9.1184000e-01 1.7871000e+00 6.8317000e-03 -9.0921000e-02 /
CHEB / -6.8819000e-01 5.8647000e-01 1.4644000e-01 -6.8578000e-02 /
CHEB / -3.6025000e-01 1.3501000e-01 8.7118000e-02 -1.4010000e-02 /

C3H5OJ(13)+H(+m)=CH3+C2H3O-1(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = 7.9976789130668315
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.9093000e+00 -1.1401000e+00 -3.3456000e-01 -1.6873000e-02 /
CHEB / 4.4324000e+00 1.0466000e+00 2.1951000e-01 -2.5266000e-02 /
CHEB / 2.6470000e-01 1.7213000e-01 1.0927000e-01 1.2709000e-02 /
CHEB / -4.2462000e-02 -3.5541000e-02 2.1340000e-02 1.9911000e-02 /

C3H5O-enol2+H(+m)=C3H5OJ(13)+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) =
5.879290683233506 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.3473000e+00 -1.5438000e+00 -3.6452000e-01 1.6484000e-03 /
CHEB / 4.3529000e+00 1.3659000e+00 1.9685000e-01 -4.9203000e-02 /
CHEB / 3.3458000e-01 2.4454000e-01 1.2682000e-01 5.3680000e-03 /
CHEB / -3.8946000e-02 -3.5741000e-02 3.5887000e-02 1.8087000e-02 /

C3H5OJ(17)+H(+m)=C3H5OJ(13)+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
14.91852274503698 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.3463000e+00 -9.2035000e-01 -3.0681000e-01 -2.1258000e-02 /
CHEB / 1.6071000e+00 8.5163000e-01 2.1478000e-01 -2.0456000e-02 /
CHEB / 2.4453000e-01 1.4737000e-01 1.0114000e-01 2.0105000e-02 /
CHEB / -2.2461000e-02 -3.2722000e-02 1.3065000e-02 1.9477000e-02 /

pC3H5+OH(+m)=C3H5OJ(13)+H(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -16.55419145128218
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 4    4 /
CHEB / 8.4981000e+00 -8.4885000e-01 -2.9585000e-01 -2.2344000e-02 /
CHEB / 1.4573000e+00 7.9141000e-01 2.1273000e-01 -1.9305000e-02 /
CHEB / 2.1613000e-01 1.3583000e-01 9.7182000e-02 2.3236000e-02 /
CHEB / -2.3403000e-02 -3.2844000e-02 9.6898000e-03 1.8925000e-02 /

CH3CHcOH+H(+m)=C3H5OJ(13)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -17.118298231669556
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.5552000e+00 -8.6285000e-01 -2.9804000e-01 -2.2107000e-02 /
CHEB / 1.4230000e+00 8.0306000e-01 2.1309000e-01 -1.9573000e-02 /
CHEB / 2.2165000e-01 1.3824000e-01 9.8045000e-02 2.2611000e-02 /
CHEB / -2.1676000e-02 -3.2769000e-02 1.0386000e-02 1.9057000e-02 /

C3H5OJ(12)+H(+m)=C3H5OJ(13)+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) =
6.079220264716518 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.3910000e+00 -5.1386000e-01 -1.8656000e-01 -2.1986000e-02 /
CHEB / 3.6140000e+00 5.2131000e-01 1.7012000e-01 5.3693000e-03 /
CHEB / 3.5479000e-01 4.7850000e-02 3.4567000e-02 1.8003000e-02 /
CHEB / 5.2958000e-02 -3.9574000e-02 -1.0346000e-02 1.4778000e-03 /

C3H5OJ(13)+H(+m)=CH3+CH2CHO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -15.492905856823944
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2618000e+01 -5.1231000e-01 -2.0984000e-01 -2.1759000e-02 /
CHEB / 5.0671000e-01 5.1358000e-01 1.8740000e-01 -6.3502000e-04 /
CHEB / 1.0073000e-01 6.6356000e-02 4.7987000e-02 2.1543000e-02 /
CHEB / 3.1803000e-03 -4.1936000e-02 -9.5718000e-03 6.6780000e-03 /

C2H5+HCO(+m)=C3H6O(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O) High-P Limit: R_Recombination exact:  [
C_rad/H2/Cs , CO_pri_rad ]    deltaHrxn(T=298K) = -82.88255514346132
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2904000e+01 3.7506000e-01 -5.3725000e-02 3.6058000e-03 /
CHEB / -8.6157000e-01 6.0208000e-01 -5.8219000e-02 -4.7675000e-03 /
CHEB / -5.4759000e-01 3.4118000e-01 1.3930000e-03 -9.1741000e-03 /
CHEB / -3.1094000e-01 1.4034000e-01 2.1511000e-02 -2.7802000e-03 /

C2H5+HCO(+m)=C3H6O-enol(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -75.86315817783101
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0505000e+01 -1.0518000e+00 -1.5848000e-01 1.6149000e-02 /
CHEB / 4.8649000e-01 1.4310000e+00 -1.4888000e-01 -1.5632000e-02 /
CHEB / -3.1689000e-01 7.0813000e-01 2.1040000e-02 -3.1663000e-02 /
CHEB / -3.1950000e-01 2.3130000e-01 6.0095000e-02 -1.2705000e-02 /
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CH3+C2H3O-1(+m)=C2H5+HCO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -26.200809539833525
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3055000e+01 -1.1522000e+00 -3.9074000e-01 -1.7895000e-02 /
CHEB / 4.8393000e-01 1.0139000e+00 2.5086000e-01 -4.0093000e-02 /
CHEB / -2.6539000e-02 2.1150000e-01 1.2862000e-01 1.8481000e-02 /
CHEB / -8.8406000e-02 -1.8044000e-02 2.8052000e-02 2.3779000e-02 /

C3H5O-enol2+H(+m)=C2H5+HCO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -12.323839943533184
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1959000e+01 -2.0319000e+00 -3.3459000e-01 3.2593000e-02 /
CHEB / 1.5127000e+00 1.7018000e+00 8.4830000e-02 -8.0075000e-02 /
CHEB / 1.2626000e-01 3.9155000e-01 1.5551000e-01 -1.3762000e-02 /
CHEB / -1.0571000e-01 -2.3820000e-02 6.5331000e-02 1.6450000e-02 /

C3H5OJ(17)+H(+m)=C2H5+HCO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -33.121653371803674
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2299000e+01 -8.7654000e-01 -3.4579000e-01 -3.3467000e-02 /
CHEB / 2.8175000e-01 7.9429000e-01 2.4412000e-01 -2.1138000e-02 /
CHEB / -8.8380000e-02 1.5974000e-01 1.1282000e-01 2.8382000e-02 /
CHEB / -1.0386000e-01 -1.8710000e-02 1.6964000e-02 2.2427000e-02 /

pC3H5+OH(+m)=C2H5+HCO(+m)           1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -34.75732207804887 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2352000e+01 -7.9450000e-01 -3.2868000e-01 -3.6623000e-02 /
CHEB / 1.9665000e-01 7.3130000e-01 2.4048000e-01 -1.6328000e-02 /
CHEB / -1.0977000e-01 1.4245000e-01 1.0625000e-01 3.1405000e-02 /
CHEB / -1.0734000e-01 -2.0669000e-02 1.2662000e-02 2.1862000e-02 /

CH3CHcOH+H(+m)=C2H5+HCO(+m)         1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -35.32142885843625 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2428000e+01 -8.1032000e-01 -3.3207000e-01 -3.6031000e-02 /
CHEB / 1.5015000e-01 7.4334000e-01 2.4117000e-01 -1.7276000e-02 /
CHEB / -1.0567000e-01 1.4589000e-01 1.0762000e-01 3.0821000e-02 /
CHEB / -1.0515000e-01 -2.0215000e-02 1.3541000e-02 2.1992000e-02 /

C3H5OJ(12)+H(+m)=C2H5+HCO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -12.123910362050172
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3168000e+01 -8.6990000e-01 -1.8690000e-01 1.4938000e-02 /
CHEB / 5.6253000e-01 7.9606000e-01 1.1022000e-01 -4.0502000e-02 /
CHEB / 6.3197000e-02 1.5186000e-01 7.5279000e-02 1.1315000e-02 /
CHEB / -4.7635000e-02 -3.8622000e-02 1.2588000e-02 1.1145000e-02 /
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CH3+CH2CHO(+m)=C2H5+HCO(+m)         1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -2.7102247699427444 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1638000e+01 -1.1644000e+00 -1.0703000e-01 9.5122000e-03 /
CHEB / 1.3820000e+00 9.9531000e-01 -4.1504000e-03 -2.3388000e-02 /
CHEB / 8.1912000e-02 2.6115000e-01 8.2409000e-02 -5.4252000e-03 /
CHEB / -7.9521000e-02 -2.6444000e-02 3.7047000e-02 1.1136000e-02 /

C3H5OJ(13)+H(+m)=C2H5+HCO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -18.20313062676669
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3765000e+01 -5.1552000e-01 -2.1463000e-01 -2.2215000e-02 /
CHEB / 2.2224000e-01 5.0812000e-01 1.8857000e-01 -9.8280000e-04 /
CHEB / 2.5295000e-02 7.4145000e-02 5.0703000e-02 2.1356000e-02 /
CHEB / -1.7891000e-02 -3.8924000e-02 -7.9995000e-03 7.3773000e-03 /

C3H5OJ(8)+H(+m)=C3H6O(+m)                         1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O) High-P Limit:
R_Recombination estimate: (Average:) [ CO_rad/NonDe , H_rad ]
      deltaHrxn(T=298K) = -88.98691178253537 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2325000e+01 6.1971000e-01 -1.2790000e-01 2.1916000e-02 /
CHEB / -1.0499000e+00 7.8759000e-01 -6.2174000e-02 -1.6950000e-02 /
CHEB / -6.4879000e-01 3.5919000e-01 2.4222000e-02 -1.1846000e-02 /
CHEB / -3.3201000e-01 1.2035000e-01 2.7974000e-02 1.8741000e-03 /

C3H5OJ(8)+H(+m)=C3H6O-enol(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
81.96751481690507 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0262000e+01 -7.2106000e-01 -2.6339000e-01 4.1320000e-02 /
CHEB / 4.8115000e-02 1.6316000e+00 -1.4111000e-01 -3.8432000e-02 /
CHEB / -4.6011000e-01 6.9429000e-01 5.7297000e-02 -3.9369000e-02 /
CHEB / -3.3205000e-01 2.0052000e-01 6.7391000e-02 -9.5629000e-03 /

CH3+C2H3O-1(+m)=C3H5OJ(8)+H(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -20.096452900759473
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.3514000e+00 -1.1580000e+00 -3.7330000e-01 -1.7954000e-02 /
CHEB / 1.3159000e+00 1.0257000e+00 2.4023000e-01 -3.4006000e-02 /
CHEB / 1.6913000e-01 2.0484000e-01 1.2205000e-01 1.6020000e-02 /
CHEB / -3.6531000e-02 -2.3092000e-02 2.5816000e-02 2.2015000e-02 /

C3H5O-enol2+H(+m)=C3H5OJ(8)+H(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -
6.219483304459139 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.9542000e+00 -1.9425000e+00 -3.3653000e-01 2.5949000e-02 /
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CHEB / 2.5850000e+00 1.6720000e+00 1.0672000e-01 -7.4980000e-02 /
CHEB / 3.2392000e-01 3.3952000e-01 1.5323000e-01 -6.4932000e-03 /
CHEB / -5.7138000e-02 -3.5616000e-02 5.6186000e-02 1.7762000e-02 /

C3H5OJ(17)+H(+m)=C3H5OJ(8)+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -27.01729673272962
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.6769000e+00 -8.9554000e-01 -3.3327000e-01 -2.9359000e-02 /
CHEB / 1.0636000e+00 8.1082000e-01 2.3300000e-01 -2.0510000e-02 /
CHEB / 1.0029000e-01 1.5927000e-01 1.0890000e-01 2.5096000e-02 /
CHEB / -5.0899000e-02 -2.1797000e-02 1.6037000e-02 2.1119000e-02 /

pC3H5+OH(+m)=C3H5OJ(8)+H(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -28.652965438974817
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.7546000e+00 -8.1608000e-01 -3.1804000e-01 -3.1674000e-02 /
CHEB / 9.6471000e-01 7.4853000e-01 2.2967000e-01 -1.7212000e-02 /
CHEB / 7.6589000e-02 1.4322000e-01 1.0323000e-01 2.8208000e-02 /
CHEB / -5.4108000e-02 -2.3128000e-02 1.2148000e-02 2.0611000e-02 /

CH3CHcOH+H(+m)=C3H5OJ(8)+H(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -29.217072219362194
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.8259000e+00 -8.3145000e-01 -3.2106000e-01 -3.1227000e-02 /
CHEB / 9.2082000e-01 7.6047000e-01 2.3028000e-01 -1.7879000e-02 /
CHEB / 8.1146000e-02 1.4644000e-01 1.0443000e-01 2.7600000e-02 /
CHEB / -5.1961000e-02 -2.2797000e-02 1.2948000e-02 2.0732000e-02 /

C3H5OJ(12)+H(+m)=C3H5OJ(8)+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -6.019553722976127
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.1504000e+00 -8.1648000e-01 -1.8407000e-01 9.5347000e-03 /
CHEB / 1.6461000e+00 7.8373000e-01 1.2040000e-01 -3.5345000e-02 /
CHEB / 2.9115000e-01 1.1350000e-01 7.1591000e-02 1.5520000e-02 /
CHEB / 1.1765000e-02 -4.8141000e-02 5.0306000e-03 1.0249000e-02 /

C3H5OJ(8)+H(+m)=CH3+CH2CHO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -3.3941318691312983
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0559000e+01 -1.0388000e+00 -1.3726000e-01 1.3504000e-02 /
CHEB / 1.5302000e+00 9.5629000e-01 3.9159000e-02 -3.3210000e-02 /
CHEB / 1.4756000e-01 1.8821000e-01 9.1276000e-02 1.7867000e-03 /
CHEB / -4.5768000e-02 -4.8368000e-02 2.4926000e-02 1.4223000e-02 /

C3H5OJ(13)+H(+m)=C3H5OJ(8)+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -12.098773987692638
kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9275000e+00 -5.0642000e-01 -2.0467000e-01 -2.1558000e-02 /
CHEB / 1.1588000e+00 5.1744000e-01 1.8615000e-01 4.6414000e-06 /
CHEB / 2.5454000e-01 5.6791000e-02 4.4863000e-02 2.1774000e-02 /
CHEB / 4.6070000e-02 -4.4715000e-02 -1.1221000e-02 5.8513000e-03 /

C3H5OJ(8)+H(+m)=C2H5+HCO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -6.1043566390740445
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1885000e+01 -1.0834000e+00 -1.2963000e-01 1.3597000e-02 /
CHEB / 1.0929000e+00 9.6554000e-01 2.5578000e-02 -3.1420000e-02 /
CHEB / 8.0324000e-02 2.1788000e-01 8.8448000e-02 -1.1367000e-03 /
CHEB / -6.5341000e-02 -3.8734000e-02 3.0057000e-02 1.3209000e-02 /

C3H6O(+m)=C2H6+CO(+m)                    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -1.955983766072542
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.1832000e+01 4.0363000e-01 -6.0971000e-02 5.1122000e-03 /
CHEB / 2.5518000e+01 6.3346000e-01 -6.1420000e-02 -5.4029000e-03 /
CHEB / -4.9261000e-01 3.4703000e-01 4.2489000e-03 -9.8640000e-03 /
CHEB / -3.0369000e-01 1.3765000e-01 2.3087000e-02 -2.2992000e-03 /

C3H6O-enol(+m)=C2H6+CO(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -8.975380731702849
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -2.0994000e+01 -1.0099000e+00 -1.7040000e-01 1.8779000e-02 /
CHEB / 2.4594000e+01 1.4661000e+00 -1.5045000e-01 -1.7937000e-02 /
CHEB / -2.9630000e-01 7.0821000e-01 2.6462000e-02 -3.3116000e-02 /
CHEB / -3.1921000e-01 2.2621000e-01 6.1663000e-02 -1.2226000e-02 /

CH3+C2H3O-1(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -111.03934844936738
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.3331000e+00 -1.1535000e+00 -3.8782000e-01 -1.7950000e-02 /
CHEB / 1.4380000e+00 1.0157000e+00 2.4902000e-01 -3.8964000e-02 /
CHEB / 1.8635000e-01 2.1064000e-01 1.2749000e-01 1.8041000e-02 /
CHEB / -2.6488000e-02 -1.8813000e-02 2.7663000e-02 2.3450000e-02 /

C3H5O-enol2+H(+m)=C2H6+CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -97.16237885306704
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.1929000e+00 -2.0193000e+00 -3.3460000e-01 3.1615000e-02 /
CHEB / 2.5001000e+00 1.6988000e+00 8.8003000e-02 -7.9388000e-02 /
CHEB / 3.4065000e-01 3.8359000e-01 1.5526000e-01 -1.2552000e-02 /
CHEB / -4.4160000e-02 -2.6172000e-02 6.3901000e-02 1.6734000e-02 /
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C3H5OJ(17)+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -117.96019228133754
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.5900000e+00 -8.7994000e-01 -3.4366000e-01 -3.2775000e-02 /
CHEB / 1.2285000e+00 7.9689000e-01 2.4213000e-01 -2.0992000e-02 /
CHEB / 1.2337000e-01 1.5980000e-01 1.1213000e-01 2.7795000e-02 /
CHEB / -4.1838000e-02 -1.9146000e-02 1.6817000e-02 2.2185000e-02 /

pC3H5+OH(+m)=C2H6+CO(+m)            1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -119.59586098758272 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.6467000e+00 -7.9831000e-01 -3.2686000e-01 -3.5775000e-02 /
CHEB / 1.1413000e+00 7.3403000e-01 2.3854000e-01 -1.6461000e-02 /
CHEB / 1.0161000e-01 1.4269000e-01 1.0572000e-01 3.0835000e-02 /
CHEB / -4.5291000e-02 -2.1002000e-02 1.2592000e-02 2.1632000e-02 /

CH3CHcOH+H(+m)=C2H6+CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -120.15996776797012 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.7221000e+00 -8.1406000e-01 -3.3019000e-01 -3.5211000e-02 /
CHEB / 1.0952000e+00 7.4605000e-01 2.3921000e-01 -1.7357000e-02 /
CHEB / 1.0579000e-01 1.4610000e-01 1.0706000e-01 3.0247000e-02 /
CHEB / -4.3098000e-02 -2.0568000e-02 1.3457000e-02 2.1760000e-02 /

C3H5OJ(12)+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -96.96244927158403
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.4007000e+00 -8.6280000e-01 -1.8625000e-01 1.4184000e-02 /
CHEB / 1.5504000e+00 7.9558000e-01 1.1156000e-01 -3.9816000e-02 /
CHEB / 2.8214000e-01 1.4627000e-01 7.4850000e-02 1.1974000e-02 /
CHEB / 1.5777000e-02 -4.0534000e-02 1.1464000e-02 1.1085000e-02 /

CH3+CH2CHO(+m)=C2H6+CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -87.54876367947661 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.8221000e+00 -1.1484000e+00 -1.1037000e-01 9.9296000e-03 /
CHEB / 2.4148000e+00 9.9428000e-01 4.7045000e-04 -2.4478000e-02 /
CHEB / 2.9449000e-01 2.5011000e-01 8.4496000e-02 -4.6724000e-03 /
CHEB / -1.5561000e-02 -3.0970000e-02 3.5612000e-02 1.1677000e-02 /

C3H5OJ(13)+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -103.04166953630055
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0024000e+01 -5.1470000e-01 -2.1307000e-01 -2.2040000e-02 /
CHEB / 1.1905000e+00 5.1007000e-01 1.8818000e-01 -8.9186000e-04 /
CHEB / 2.4353000e-01 7.1730000e-02 4.9837000e-02 2.1413000e-02 /
CHEB / 4.6105000e-02 -3.9936000e-02 -8.5137000e-03 7.1558000e-03 /
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C2H5+HCO(+m)=C2H6+CO(+m)            1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O)  deltaHrxn(T=298K) = -84.83853890953387 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.6933000e+00 -1.2058000e+00 -9.6504000e-02 7.5348000e-03 /
CHEB / 2.8343000e+00 1.0006000e+00 -1.6926000e-02 -1.9644000e-02 /
CHEB / 2.8549000e-01 2.8768000e-01 7.6726000e-02 -7.0662000e-03 /
CHEB / -4.0654000e-02 -1.6000000e-02 4.0203000e-02 9.7406000e-03 /

C3H5OJ(8)+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O)   deltaHrxn(T=298K) = -90.94289554860791
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.0872000e+00 -1.0699000e+00 -1.3179000e-01 1.3547000e-02 /
CHEB / 2.1077000e+00 9.6376000e-01 2.9531000e-02 -3.1942000e-02 /
CHEB / 2.9691000e-01 2.0849000e-01 8.9504000e-02 -2.6055000e-04 /
CHEB / -1.8786000e-03 -4.2197000e-02 2.8524000e-02 1.3560000e-02 /

!PDepNetwork C3H6O-enol2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     CH2CHCH2O         25.06 72.63 18.45 22.37 25.85 28.76 33.26 36.56
      41.63
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+CH2OH=C3H6O-enol2  1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+OH=C3H6O-enol2    1.4157154e+13      -0.15000
2.9166667e+02
!     C3H5O-enol2+H=C3H6O-enol2     5.0000000e+13      0.00000
0.0000000e+00
!     CH2CHCH2O+H=C3H6O-enol2       1.4157154e+13      -0.15000
2.9166667e+02

C2H3+CH2OH(+m)=C3H6O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     C_rad/H2/O      deltaHrxn(T=298K) = -
97.28020081892926 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1832000e+01 8.5172000e-01 -1.9300000e-01 /
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CHEB / -1.7262000e+00 1.2345000e+00 -1.6008000e-01 /
CHEB / -1.1575000e+00 6.9781000e-01 -6.1210000e-03 /
CHEB / -7.0629000e-01 3.0293000e-01 4.8210000e-02 /
CHEB / -4.0554000e-01 9.3030000e-02 4.0506000e-02 /

C2H3+CH2OH(+m)=aC3H5+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = -17.628206949731894
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1298000e+01 -1.2542000e+00 -1.0995000e-01 /
CHEB / 7.2483000e-01 9.8733000e-01 -2.1792000e-02 /
CHEB / 4.4279000e-02 3.8543000e-01 8.5273000e-02 /
CHEB / -1.3511000e-01 3.0359000e-02 6.9614000e-02 /
CHEB / -1.0859000e-01 -7.4307000e-02 1.5338000e-02 /

C2H3+CH2OH(+m)=C3H5O-enol2+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = -17.638473776874143
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0747000e+01 -1.2573000e+00 -1.0991000e-01 /
CHEB / 1.3961000e+00 9.8514000e-01 -2.2455000e-02 /
CHEB / 2.1782000e-01 3.8813000e-01 8.4563000e-02 /
CHEB / -7.2801000e-02 3.3416000e-02 6.9988000e-02 /
CHEB / -8.4025000e-02 -7.3182000e-02 1.6220000e-02 /

aC3H5+OH(+m)=C3H6O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     O_pri_rad      deltaHrxn(T=298K) = -
79.65199386919737 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2317000e+01 3.3343000e-01 -3.5123000e-02 /
CHEB / -9.6947000e-01 6.0764000e-01 -5.5748000e-02 /
CHEB / -7.3531000e-01 4.5797000e-01 -2.2439000e-02 /
CHEB / -5.2787000e-01 2.8053000e-01 9.0861000e-03 /
CHEB / -3.4662000e-01 1.3239000e-01 2.4725000e-02 /

C3H5O-enol2+H(+m)=C3H6O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeO     H_rad       deltaHrxn(T=298K) = -
79.64172704205511 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3341000e+01 3.1976000e-01 -3.2540000e-02 /
CHEB / -8.8941000e-01 5.8455000e-01 -5.1986000e-02 /
CHEB / -6.8736000e-01 4.4451000e-01 -2.1507000e-02 /
CHEB / -5.0311000e-01 2.7626000e-01 8.0572000e-03 /
CHEB / -3.3098000e-01 1.3326000e-01 2.3500000e-02 /

C3H5O-enol2+H(+m)=aC3H5+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = 0.010266827142249468
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0183000e+01 -1.4606000e+00 -5.0493000e-02 /
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CHEB / 2.9514000e+00 9.0850000e-01 -5.9590000e-02 /
CHEB / 3.0888000e-01 5.2705000e-01 1.7254000e-02 /
CHEB / -2.0548000e-01 1.7275000e-01 5.7273000e-02 /
CHEB / -1.7826000e-01 -2.1168000e-02 4.4958000e-02 /

CH2CHCH2O+H(+m)=C3H6O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
106.07907041158106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1122000e+01 1.5260000e+00 -4.6444000e-01 /
CHEB / -2.0386000e+00 1.5278000e+00 -1.3288000e-01 /
CHEB / -1.3515000e+00 7.4508000e-01 3.9140000e-02 /
CHEB / -7.9409000e-01 2.8373000e-01 6.2809000e-02 /
CHEB / -4.3580000e-01 7.6764000e-02 3.6187000e-02 /

CH2CHCH2O+H(+m)=C2H3+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = -8.798869592651803
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0974000e+01 -9.8596000e-01 -1.7592000e-01 /
CHEB / 1.3413000e+00 9.1570000e-01 8.0055000e-02 /
CHEB / 2.3719000e-01 2.1635000e-01 1.0794000e-01 /
CHEB / -6.5008000e-02 -5.1919000e-02 3.1232000e-02 /
CHEB / -6.6251000e-02 -7.2531000e-02 -1.7713000e-02 /

CH2CHCH2O+H(+m)=aC3H5+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = -26.42707654238369
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1549000e+01 -1.0288000e+00 -1.8921000e-01 /
CHEB / 4.0320000e-01 8.8189000e-01 7.5515000e-02 /
CHEB / -4.4243000e-02 2.7294000e-01 1.0810000e-01 /
CHEB / -1.3223000e-01 -1.0996000e-02 4.5953000e-02 /
CHEB / -9.0677000e-02 -6.8903000e-02 -6.4654000e-03 /

CH2CHCH2O+H(+m)=C3H5O-enol2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (C3H6O-enol2) deltaHrxn(T=298K) = -26.43734336952594
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0978000e+01 -1.0294000e+00 -1.9021000e-01 /
CHEB / 1.0893000e+00 8.7986000e-01 7.5647000e-02 /
CHEB / 1.3108000e-01 2.7437000e-01 1.0828000e-01 /
CHEB / -7.0476000e-02 -9.2921000e-03 4.6503000e-02 /
CHEB / -6.6251000e-02 -6.8364000e-02 -5.9933000e-03 /

!PDepNetwork C3H4O
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     CHCHCHO           45.67 67.33 16.24 19.74 22.69 25.03 28.29 30.37
      33.17
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     tSPC(346)         46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41
      32.99
!     C3H3O-enone       24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05
      32.71
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     CHCHCHO+H=C3H4O         5.3600000e+14      0.00000
9.8000000e+02
!     C2H3+HCO=C3H4O          1.8100000e+13      0.00000
0.0000000e+00
!     tSPC(346)+H=C3H4O             1.4157154e+13      -0.15000
2.9166667e+02
!     C3H3O-enone+H=C3H4O           1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4+CO=C3H4O           4.0416992e+07      1.70125
8.2775000e+04

C3H4O(+m)=C2H4+CO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H4O)  deltaHrxn(T=298K) = 1.3098123118801546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0276000e+01 3.3011000e-01 -4.2359000e-02 /
CHEB / 2.7685000e+01 5.6708000e-01 -5.9544000e-02 /
CHEB / -8.2414000e-01 3.6227000e-01 -1.4123000e-02 /
CHEB / -5.2190000e-01 1.6827000e-01 1.3428000e-02 /
CHEB / -2.9646000e-01 4.9688000e-02 1.6009000e-02 /

CHCHCHO+H(+m)=C3H4O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H4O) High-P Limit: R_Recombination exact:  Cd_pri_rad     H_rad
      deltaHrxn(T=298K) = -111.95810092523142 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7411000e+00 4.3769000e+00 -4.6877000e-01 /
CHEB / -1.7294000e+00 4.1353000e-01 -3.2372000e-02 /
CHEB / -1.1730000e+00 1.9790000e-01 3.9297000e-02 /
CHEB / -5.6178000e-01 6.1501000e-02 1.3629000e-02 /
CHEB / -2.6199000e-01 1.4719000e-02 4.6316000e-03 /

CHCHCHO+H(+m)=C2H3+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -15.488093927699003 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4499000e+01 -8.1063000e-02 -5.8006000e-02 /
CHEB / 2.3150000e-01 8.6507000e-02 6.1949000e-02 /
CHEB / 2.8559000e-02 9.9786000e-03 6.7480000e-03 /
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CHEB / 3.1796000e-02 -1.2317000e-02 -8.3486000e-03 /
CHEB / 2.4233000e-02 -4.8864000e-03 -3.4582000e-03 /

CHCHCHO+H(+m)=tSPC(346)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = 0.7798775256041495 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2125000e+00 -6.7790000e-02 -4.3921000e-02 /
CHEB / 2.6118000e+00 8.2387000e-02 5.3115000e-02 /
CHEB / 5.7690000e-01 -5.5163000e-03 -3.3179000e-03 /
CHEB / 1.8325000e-01 -9.7261000e-03 -6.1302000e-03 /
CHEB / 6.9861000e-02 -1.0229000e-03 -7.9684000e-04 /

CHCHCHO+H(+m)=C3H3O-enone+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -21.147797504258115 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1571000e+01 -6.7292000e-02 -5.3826000e-02 /
CHEB / 6.3595000e-01 6.9866000e-02 5.5797000e-02 /
CHEB / 8.4977000e-02 1.1333000e-02 8.5737000e-03 /
CHEB / 5.1318000e-02 -1.0377000e-02 -7.5925000e-03 /
CHEB / 3.5664000e-02 -4.9087000e-03 -3.7827000e-03 /

CHCHCHO+H(+m)=C2H4+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -110.64828861335127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3047000e+01 -5.2754000e-02 -4.8952000e-02 /
CHEB / 3.4234000e-01 5.5067000e-02 5.0258000e-02 /
CHEB / -3.4925000e-02 1.0201000e-02 9.0711000e-03 /
CHEB / 4.4345000e-03 -9.2240000e-03 -7.1415000e-03 /
CHEB / 1.8247000e-02 -4.5919000e-03 -3.9029000e-03 /

C2H3+HCO(+m)=C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H4O) High-P Limit: R_Recombination exact:  Cd_pri_rad
CO_pri_rad        deltaHrxn(T=298K) = -96.47000699753242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2067000e+01 1.0577000e+00 -2.8588000e-01 /
CHEB / -1.7843000e+00 1.0074000e+00 -5.9452000e-02 /
CHEB / -1.0654000e+00 4.0776000e-01 2.7253000e-02 /
CHEB / -5.5171000e-01 1.1531000e-01 2.5797000e-02 /
CHEB / -2.8068000e-01 2.0700000e-02 8.6607000e-03 /

C2H3+HCO(+m)=C3H3O-enone+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -5.659703576559117 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0149000e+01 -9.0850000e-01 -1.4949000e-01 /
CHEB / 7.9393000e-01 9.0066000e-01 9.0928000e-02 /
CHEB / 5.5773000e-02 1.3602000e-01 7.5854000e-02 /
CHEB / -2.8959000e-02 -6.9009000e-02 7.8092000e-03 /
CHEB / -6.0028000e-03 -5.0885000e-02 -1.4539000e-02 /

C2H3+HCO(+m)=C2H4+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -95.16019468565227 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.1977000e+01 -9.6048000e-01 -1.5383000e-01 /
CHEB / 2.7404000e-01 9.0042000e-01 8.2813000e-02 /
CHEB / -1.0359000e-01 1.8252000e-01 7.9109000e-02 /
CHEB / -8.5875000e-02 -5.0338000e-02 1.6377000e-02 /
CHEB / -3.1209000e-02 -5.3542000e-02 -1.1206000e-02 /

tSPC(346)+H(+m)=C3H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/OneDe     H_rad         deltaHrxn(T=298K) = -
112.73797845083557 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7720000e+00 4.4905000e+00 -4.3369000e-01 /
CHEB / -1.9912000e+00 4.0262000e-01 -4.7922000e-02 /
CHEB / -1.2034000e+00 1.9121000e-01 3.5209000e-02 /
CHEB / -5.7726000e-01 6.0211000e-02 1.2912000e-02 /
CHEB / -2.7491000e-01 1.4587000e-02 4.5481000e-03 /

tSPC(346)+H(+m)=C2H3+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -16.267971453303154 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2725000e+01 -6.8997000e-02 -5.0488000e-02 /
CHEB / -4.3108000e-02 7.3328000e-02 5.3789000e-02 /
CHEB / -2.1870000e-03 9.0363000e-03 6.1847000e-03 /
CHEB / 1.6694000e-02 -1.0673000e-02 -7.4525000e-03 /
CHEB / 1.1236000e-02 -4.2692000e-03 -3.0617000e-03 /

tSPC(346)+H(+m)=C3H3O-enone+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -21.927675029862264 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7832000e+00 -5.5317000e-02 -4.5687000e-02 /
CHEB / 3.6980000e-01 5.7345000e-02 4.7338000e-02 /
CHEB / 5.6547000e-02 9.7533000e-03 7.5619000e-03 /
CHEB / 3.6662000e-02 -8.8746000e-03 -6.7344000e-03 /
CHEB / 2.2726000e-02 -4.1670000e-03 -3.2874000e-03 /

tSPC(346)+H(+m)=C2H4+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -111.42816613895542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1251000e+01 -4.1148000e-02 -4.0372000e-02 /
CHEB / 8.0915000e-02 4.3224000e-02 4.1591000e-02 /
CHEB / -6.1682000e-02 8.3062000e-03 7.7474000e-03 /
CHEB / -9.6909000e-03 -7.8375000e-03 -6.3310000e-03 /
CHEB / 5.4770000e-03 -3.7962000e-03 -3.3467000e-03 /

C3H3O-enone+H(+m)=C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/OneDe     H_rad         deltaHrxn(T=298K) = -
90.8103034209733 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1876000e+01 5.2109000e-01 -9.5123000e-02 /
CHEB / -1.2980000e+00 7.8692000e-01 -9.0982000e-02 /
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CHEB / -9.3029000e-01 4.1316000e-01 -1.5134000e-03 /
CHEB / -5.3052000e-01 1.5088000e-01 2.4026000e-02 /
CHEB / -2.8184000e-01 3.2279000e-02 1.4784000e-02 /

C3H3O-enone+H(+m)=C2H4+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O)  deltaHrxn(T=298K) = -89.50049110909315 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0850000e+01 -1.2427000e+00 -7.5758000e-02 /
CHEB / 9.5508000e-01 1.0154000e+00 -1.4687000e-02 /
CHEB / -1.0296000e-01 3.3585000e-01 6.3952000e-02 /
CHEB / -1.7524000e-01 -3.9348000e-03 3.7070000e-02 /
CHEB / -7.4873000e-02 -6.3329000e-02 1.4054000e-03 /

!PDepNetwork C3H4O-enone
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H4O-enone       -13.82      68.58 16.45 19.54 22.36 24.81 28.75
      31.71 36.31
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HCCO        37.64 58.8  11.97 13.09 13.94 14.64 15.74 16.57 17.91
!     C3H3O-enone       24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05
      32.71
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H3OJ            41.87 70.08 16.16 18.35 20.4  22.25 25.39 27.81
      31.6  null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+HCCO=C3H4O-enone    7.2300000e+13      0.00000
0.0000000e+00
!     C3H3O-enone+H=C3H4O-enone     5.0000000e+13      0.00000
0.0000000e+00
!     C3H3OJ+H=C3H4O-enone    1.4157154e+13      -0.15000
2.9166667e+02

CH3+HCCO(+m)=C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone) High-P Limit: R_Recombination exact:
C_methyl     Cd_pri_rad       deltaHrxn(T=298K) = -86.70053638484191
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3087000e+01 5.9357000e-01 -7.5770000e-02 /
CHEB / -1.7065000e+00 8.0235000e-01 -2.2275000e-02 /
CHEB / -1.0342000e+00 3.4492000e-01 4.0768000e-02 /
CHEB / -5.3729000e-01 8.3768000e-02 3.1545000e-02 /
CHEB / -2.6944000e-01 -3.9304000e-03 8.4008000e-03 /

C3H3O-enone+H(+m)=C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
90.4302922107408 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.2532000e+01 9.1949000e-01 -1.9092000e-01 /
CHEB / -1.8742000e+00 8.8772000e-01 1.7044000e-02 /
CHEB / -1.1116000e+00 3.2932000e-01 5.8490000e-02 /
CHEB / -5.8086000e-01 6.5577000e-02 2.9836000e-02 /
CHEB / -2.8245000e-01 -8.6617000e-03 4.9010000e-03 /

C3H3O-enone+H(+m)=CH3+HCCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone)  deltaHrxn(T=298K) = -3.7297558258988843
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3086000e+01 -8.4677000e-01 -1.4846000e-01 /
CHEB / 7.6537000e-01 9.0679000e-01 1.0369000e-01 /
CHEB / 2.2017000e-02 7.4871000e-02 7.5551000e-02 /
CHEB / -5.8722000e-02 -9.6174000e-02 -4.6209000e-03 /
CHEB / -7.9819000e-03 -4.6443000e-02 -2.0763000e-02 /

C3H3OJ+H(+m)=C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
107.78142147617254 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7262000e+00 4.9156000e+00 -1.8726000e-01 /
CHEB / -2.4875000e+00 2.5442000e-01 1.9128000e-01 /
CHEB / -1.3634000e+00 5.8815000e-02 5.3860000e-02 /
CHEB / -6.2369000e-01 -2.3340000e-03 8.0785000e-03 /
CHEB / -2.8138000e-01 -1.1022000e-02 -5.8329000e-04 /

C3H3OJ+H(+m)=CH3+HCCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone)  deltaHrxn(T=298K) = -21.08088509133062
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2618000e+01 -5.6769000e-02 -4.3398000e-02 /
CHEB / 7.3720000e-02 6.9890000e-02 5.2980000e-02 /
CHEB / -8.0253000e-03 -4.9882000e-03 -3.1452000e-03 /
CHEB / 2.3073000e-02 -8.9662000e-03 -6.9251000e-03 /
CHEB / 1.6756000e-02 -1.0654000e-03 -9.9358000e-04 /

C3H3OJ+H(+m)=C3H3O-enone+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (C3H4O-enone)  deltaHrxn(T=298K) = -17.35112926543173
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5743000e+00 -6.2782000e-02 -4.6085000e-02 /
CHEB / 7.6911000e-01 7.6920000e-02 5.6095000e-02 /
CHEB / 1.9621000e-01 -5.2528000e-03 -3.2746000e-03 /
CHEB / 9.4276000e-02 -9.6983000e-03 -7.2167000e-03 /
CHEB / 4.2892000e-02 -1.1598000e-03 -1.0073000e-03 /

!PDepNetwork C3H8
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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!     C3H8              -24.27      66.07 17.76 22.39 26.7  30.47 36.6
      41.32 48.85
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C2H5=C3H8           3.3700000e+13      0.00000
0.0000000e+00
!     C3H7-1+H=C3H8           1.0000000e+14      0.00000
0.0000000e+00
!     C3H7-2+H=C3H8           2.0000000e+13      0.00000
0.0000000e+00

CH3+C2H5(+m)=C3H8(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#15 (C3H8) High-P Limit: R_Recombination exact:  C_methyl
C_rad/H2/Cs       deltaHrxn(T=298K) = -88.9404528831996 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2800000e+01 4.4696000e-01 -4.0634000e-02 /
CHEB / -1.3721000e+00 7.4869000e-01 -4.3724000e-02 /
CHEB / -1.0362000e+00 4.5157000e-01 1.1316000e-02 /
CHEB / -6.3686000e-01 1.8814000e-01 3.3795000e-02 /
CHEB / -3.6932000e-01 3.9430000e-02 2.4578000e-02 /

C3H7-1+H(+m)=C3H8(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#15 (C3H8) High-P Limit: R_Recombination exact:  C_rad/H2/Cs     H_rad
      deltaHrxn(T=298K) = -101.56908729212464 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2548000e+01 1.3080000e+00 -3.5794000e-01 /
CHEB / -2.0335000e+00 1.0163000e+00 5.5360000e-02 /
CHEB / -1.3080000e+00 4.6137000e-01 7.2572000e-02 /
CHEB / -7.2794000e-01 1.2770000e-01 4.5963000e-02 /
CHEB / -3.8237000e-01 4.6078000e-03 1.4897000e-02 /

C3H7-1+H(+m)=CH3+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #15 (C3H8)  deltaHrxn(T=298K) = -12.628634408925034 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3424000e+01 -8.7474000e-01 -1.8469000e-01 /
CHEB / 6.5907000e-01 8.6048000e-01 1.2610000e-01 /
CHEB / 1.1340000e-01 1.6686000e-01 8.6649000e-02 /
CHEB / -3.8971000e-02 -8.0961000e-02 9.0371000e-03 /
CHEB / -2.4445000e-02 -6.9714000e-02 -2.3068000e-02 /

C3H7-2+H(+m)=C3H8(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#15 (C3H8) High-P Limit: R_Recombination exact:  C_rad/H/NonDeC
H_rad       deltaHrxn(T=298K) = -102.3691345834382 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.1702000e+01 1.4664000e+00 -4.1774000e-01 /
CHEB / -2.0713000e+00 1.0026000e+00 8.4992000e-02 /
CHEB / -1.3325000e+00 4.5185000e-01 8.0267000e-02 /
CHEB / -7.4496000e-01 1.2194000e-01 4.5549000e-02 /
CHEB / -3.9079000e-01 2.7909000e-03 1.3632000e-02 /

C3H7-2+H(+m)=CH3+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #15 (C3H8)  deltaHrxn(T=298K) = -13.428681700238595 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2765000e+01 -8.2557000e-01 -1.9662000e-01 /
CHEB / 5.9898000e-01 8.1669000e-01 1.4474000e-01 /
CHEB / 1.0019000e-01 1.5428000e-01 8.3213000e-02 /
CHEB / -4.4869000e-02 -7.9254000e-02 4.3984000e-03 /
CHEB / -2.8979000e-02 -6.5883000e-02 -2.3561000e-02 /

C3H7-2+H(+m)=C3H7-1+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #15 (C3H8)  deltaHrxn(T=298K) = -0.8000472913135539 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7005000e+00 -7.4313000e-01 -1.8234000e-01 /
CHEB / 2.4329000e+00 8.0952000e-01 1.4738000e-01 /
CHEB / 5.4799000e-01 5.7237000e-02 7.5576000e-02 /
CHEB / 6.9993000e-02 -9.1178000e-02 -1.2620000e-02 /
CHEB / 1.9414000e-02 -4.3724000e-02 -2.5693000e-02 /

!PDepNetwork nC4H10
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nC4H10            -28.28      76.34 25.39 30.69 35.76 40.25 47.63
      53.34 62.48
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C4H9-1            20.65 78.53 23.01 28.55 33.6  37.94 44.89 50.17
      58.56
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H9-2            18.01 78.98 21.99 27.3  32.36 36.82 44.06 49.58
      58.28
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H7-1=nC4H10       3.3700000e+13      0.00000
0.0000000e+00
!     C4H9-1+H=nC4H10         1.0000000e+14      0.00000
0.0000000e+00
!     C2H5+C2H5=nC4H10        1.1500000e+13      0.00000
0.0000000e+00
!     C4H9-2+H=nC4H10         2.0000000e+13      0.00000
0.0000000e+00
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CH3+C3H7-1(+m)=nC4H10(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10) High-P Limit: R_Recombination exact:  C_methyl
C_rad/H2/Cs       deltaHrxn(T=298K) = -88.7308931115936 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2906000e+01 4.1852000e-01 -3.0356000e-02 /
CHEB / -1.4848000e+00 7.4410000e-01 -4.1697000e-02 /
CHEB / -1.1322000e+00 5.1906000e-01 -2.2319000e-03 /
CHEB / -7.8708000e-01 2.7322000e-01 2.6864000e-02 /
CHEB / -5.0261000e-01 9.2676000e-02 3.1484000e-02 /

CH3+C3H7-1(+m)=C2H5+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -1.5995056914425518
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0779000e+01 -1.3420000e+00 -5.1018000e-02 /
CHEB / 2.5735000e+00 1.0332000e+00 -4.0719000e-02 /
CHEB / 2.3815000e-01 4.6549000e-01 4.7758000e-02 /
CHEB / -2.3098000e-01 4.1086000e-02 6.0617000e-02 /
CHEB / -1.3979000e-01 -1.0506000e-01 1.8960000e-02 /

C4H9-1+H(+m)=nC4H10(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#16 (nC4H10) High-P Limit: R_Recombination exact:  C_rad/H2/Cs     H_rad
      deltaHrxn(T=298K) = -101.01947588694458 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2924000e+01 7.1019000e-01 -1.0353000e-01 /
CHEB / -1.9095000e+00 1.0892000e+00 -7.7558000e-02 /
CHEB / -1.4072000e+00 6.1848000e-01 2.2209000e-02 /
CHEB / -8.9961000e-01 2.4455000e-01 5.3711000e-02 /
CHEB / -5.2677000e-01 4.9880000e-02 3.5930000e-02 /

C4H9-1+H(+m)=CH3+C3H7-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -12.28858277535097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2178000e+01 -1.1969000e+00 -9.1193000e-02 /
CHEB / 1.6182000e+00 1.0575000e+00 -9.0875000e-03 /
CHEB / 2.6413000e-01 3.3223000e-01 8.8315000e-02 /
CHEB / -1.0657000e-01 -4.7716000e-02 5.3012000e-02 /
CHEB / -7.3353000e-02 -1.0733000e-01 -6.1379000e-03 /

C4H9-1+H(+m)=C2H5+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -13.888088466793523
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2467000e+01 -1.2048000e+00 -8.9969000e-02 /
CHEB / 1.2349000e+00 1.0552000e+00 -1.0695000e-02 /
CHEB / 1.6528000e-01 3.4053000e-01 8.6601000e-02 /
CHEB / -1.3814000e-01 -4.2225000e-02 5.4108000e-02 /
CHEB / -8.6837000e-02 -1.0739000e-01 -4.5509000e-03 /
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C4H9-1+H(+m)=C4H9-2+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -2.639603250818574
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7695000e+00 -1.1250000e+00 -1.0605000e-01 /
CHEB / 3.1282000e+00 1.0588000e+00 9.9202000e-03 /
CHEB / 5.6166000e-01 2.6162000e-01 1.0122000e-01 /
CHEB / -1.7607000e-02 -8.0339000e-02 4.0939000e-02 /
CHEB / -2.9053000e-02 -9.9948000e-02 -1.7561000e-02 /

C2H5+C2H5(+m)=nC4H10(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     C_rad/H2/Cs         deltaHrxn(T=298K) = -
87.13138742015106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2436000e+01 3.9778000e-01 -2.6983000e-02 /
CHEB / -1.4318000e+00 7.1127000e-01 -3.7591000e-02 /
CHEB / -1.1080000e+00 5.0414000e-01 -2.6327000e-03 /
CHEB / -7.9098000e-01 2.7246000e-01 2.4514000e-02 /
CHEB / -5.0963000e-01 9.6919000e-02 3.0148000e-02 /

C4H9-2+H(+m)=nC4H10(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#16 (nC4H10) High-P Limit: R_Recombination exact:  C_rad/H/NonDeC
H_rad       deltaHrxn(T=298K) = -98.379872636126 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2439000e+01 6.1233000e-01 -7.3580000e-02 /
CHEB / -1.8815000e+00 1.0023000e+00 -7.3315000e-02 /
CHEB / -1.3488000e+00 6.0280000e-01 1.2054000e-02 /
CHEB / -8.8926000e-01 2.5675000e-01 4.7207000e-02 /
CHEB / -5.3044000e-01 5.9983000e-02 3.6442000e-02 /

C4H9-2+H(+m)=CH3+C3H7-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -9.64897952453239
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1323000e+01 -1.2421000e+00 -7.6154000e-02 /
CHEB / 1.7941000e+00 1.0655000e+00 -2.4173000e-02 /
CHEB / 2.7969000e-01 3.6848000e-01 7.9146000e-02 /
CHEB / -1.4044000e-01 -3.1712000e-02 5.7845000e-02 /
CHEB / -9.2345000e-02 -1.1124000e-01 1.6095000e-04 /

C4H9-2+H(+m)=C2H5+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (nC4H10)      deltaHrxn(T=298K) = -11.248485215974942
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1627000e+01 -1.2507000e+00 -7.4649000e-02 /
CHEB / 1.3957000e+00 1.0623000e+00 -2.5652000e-02 /
CHEB / 1.8287000e-01 3.7738000e-01 7.6888000e-02 /
CHEB / -1.7163000e-01 -2.5126000e-02 5.8627000e-02 /
CHEB / -1.0641000e-01 -1.1088000e-01 1.9383000e-03 /

!PDepNetwork iC4H10
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H10            -30.67      71.16 23.9  30.21 35.82 40.56 48.08
      53.8  63.01
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     iC4H9       19.15 76.39 23.23 28.98 34.04 38.33 45.13 50.31 58.58
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tC4H9             14.3  76.21 21.71 26.64 31.62 36.12 43.55 49.22
      58.13
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H7-2=iC4H10       6.6400000e+14      -0.57000
0.0000000e+00
!     iC4H9+H=iC4H10          1.0000000e+14      0.00000
0.0000000e+00
!     tC4H9+H=iC4H10          5.0000000e+13      0.00000
0.0000000e+00

CH3+C3H7-2(+m)=iC4H10(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (iC4H10) High-P Limit: R_Recombination exact:  C_methyl
C_rad/H/NonDeC          deltaHrxn(T=298K) = -91.9204141066212 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2702000e+01 3.9897000e-01 -2.9922000e-02 /
CHEB / -1.6688000e+00 7.0897000e-01 -4.1095000e-02 /
CHEB / -1.1026000e+00 4.9555000e-01 -2.8913000e-03 /
CHEB / -7.3782000e-01 2.6499000e-01 2.4651000e-02 /
CHEB / -4.6797000e-01 9.6854000e-02 2.8979000e-02 /

iC4H9+H(+m)=iC4H10(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#17 (iC4H10) High-P Limit: R_Recombination exact:  C_rad/H2/Cs     H_rad
      deltaHrxn(T=298K) = -101.90908448867853 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3208000e+01 5.9494000e-01 -7.7378000e-02 /
CHEB / -1.6995000e+00 9.4390000e-01 -6.4459000e-02 /
CHEB / -1.2124000e+00 5.6277000e-01 1.4771000e-02 /
CHEB / -7.7667000e-01 2.4439000e-01 4.3806000e-02 /
CHEB / -4.6386000e-01 6.6586000e-02 3.2373000e-02 /

iC4H9+H(+m)=CH3+C3H7-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (iC4H10)      deltaHrxn(T=298K) = -9.988670382057347
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2654000e+01 -1.2189000e+00 -8.5585000e-02 /
CHEB / 1.3912000e+00 1.0466000e+00 -1.3825000e-02 /
CHEB / 2.3935000e-01 3.4761000e-01 8.0522000e-02 /
CHEB / -1.1026000e-01 -2.7861000e-02 5.1991000e-02 /
CHEB / -7.9115000e-02 -9.8846000e-02 -8.7196000e-04 /
```

```
iC4H9+H(+m)=tC4H9+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#17 (iC4H10)      deltaHrxn(T=298K) = -4.849350664026865 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4063000e+00 -1.1804000e+00 -9.3653000e-02 /
CHEB / 2.7026000e+00 1.0505000e+00 -4.6912000e-03 /
CHEB / 5.3384000e-01 3.1097000e-01 8.8374000e-02 /
CHEB / -1.4618000e-02 -4.7785000e-02 4.7278000e-02 /
CHEB / -3.5690000e-02 -9.7519000e-02 -6.8036000e-03 /

tC4H9+H(+m)=iC4H10(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#17 (iC4H10) High-P Limit: R_Recombination estimate: (Average:)
C_rad/Cs3     H_rad           deltaHrxn(T=298K) = -97.05973382465166
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3028000e+01 4.7786000e-01 -4.5567000e-02 /
CHEB / -1.5348000e+00 8.2152000e-01 -5.5104000e-02 /
CHEB / -1.1316000e+00 5.3520000e-01 2.4418000e-03 /
CHEB / -7.6548000e-01 2.5932000e-01 3.3785000e-02 /
CHEB / -4.7328000e-01 8.1910000e-02 3.1900000e-02 /

tC4H9+H(+m)=CH3+C3H7-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (iC4H10)      deltaHrxn(T=298K) = -5.139319718030475
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1832000e+01 -1.2840000e+00 -6.5643000e-02 /
CHEB / 1.9184000e+00 1.0493000e+00 -3.2323000e-02 /
CHEB / 2.5344000e-01 4.0137000e-01 6.5898000e-02 /
CHEB / -1.7069000e-01 4.1365000e-04 5.7162000e-02 /
CHEB / -1.1374000e-01 -1.0061000e-01 7.9000000e-03 /

!PDepNetwork C5H10_1
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C5H10_1           -5.04 83.03 26.07 33.04 39.29 44.63 53.03 59.31
      69.0  null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     C5H9_1_4          43.96 86.44 25.3  31.68 37.38 42.23 49.87 55.57
      64.34 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     C5H9_2_4          41.31 88.16 24.53 30.27 35.8  40.73 48.68 54.67
      64.36 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
```

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!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C2H5CHCHCH2             28.12 80.44 25.2  32.04 37.96 42.95 50.72
      56.46 65.27 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C4H7-14=C5H10_1     3.3700000e+13      0.00000
0.0000000e+00
!     C5H9_1_4+H=C5H10_1            1.0000000e+14      0.00000
0.0000000e+00
!     C2H5+aC3H5=C5H10_1      1.1500000e+13      0.00000
0.0000000e+00
!     C5H9_2_4+H=C5H10_1            2.0000000e+13      0.00000
0.0000000e+00
!     C3H7-1+C2H3=C5H10_1     1.4157154e+13      -0.15000
2.9166667e+02
!     C2H5CHCHCH2+H=C5H10_1         5.0000000e+13      0.00000
0.0000000e+00

CH3+C4H7-14(+m)=C5H10_1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination exact:  C_methyl
C_rad/H2/Cs       deltaHrxn(T=298K) = -89.17054603846364 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2631000e+01 5.9082000e-01 -6.3985000e-02 /
CHEB / -1.9846000e+00 1.0199000e+00 -8.3744000e-02 /
CHEB / -1.5103000e+00 6.6190000e-01 -5.9640000e-03 /
CHEB / -1.0247000e+00 3.0667000e-01 4.2099000e-02 /
CHEB / -6.5216000e-01 7.4070000e-02 4.4566000e-02 /

CH3+C4H7-14(+m)=C2H5+aC3H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -12.668386582043674
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1524000e+01 -1.3264000e+00 -5.9782000e-02 /
CHEB / 1.8416000e+00 1.0422000e+00 -4.3105000e-02 /
CHEB / 1.7995000e-01 4.5499000e-01 5.7886000e-02 /
CHEB / -2.1895000e-01 2.8614000e-02 6.9191000e-02 /
CHEB / -1.5339000e-01 -1.1167000e-01 1.9783000e-02 /

C5H9_1_4+H(+m)=C5H10_1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -101.08918542859848
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2818000e+01 9.4403000e-01 -1.6913000e-01 /
CHEB / -2.5786000e+00 1.3683000e+00 -1.1332000e-01 /
CHEB / -1.7632000e+00 7.3500000e-01 3.0467000e-02 /
CHEB / -1.1218000e+00 2.6434000e-01 6.9699000e-02 /
CHEB / -6.7142000e-01 3.1815000e-02 4.5292000e-02 /

C5H9_1_4+H(+m)=CH3+C4H7-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -11.91863939013485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1780000e+01 -1.1266000e+00 -1.1333000e-01 /
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CHEB / 2.0317000e+00 1.0528000e+00 1.1614000e-02 /
CHEB / 3.6614000e-01 2.7222000e-01 1.0588000e-01 /
CHEB / -8.5367000e-02 -7.8190000e-02 4.6358000e-02 /
CHEB / -7.4720000e-02 -1.0368000e-01 -1.8057000e-02 /

C5H9_1_4+H(+m)=C2H5+aC3H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -24.587025972178516
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2930000e+01 -1.1817000e+00 -1.0660000e-01 /
CHEB / 8.5938000e-01 1.0411000e+00 -1.5105000e-03 /
CHEB / 7.3464000e-02 3.3160000e-01 9.6598000e-02 /
CHEB / -1.5708000e-01 -4.3132000e-02 5.7849000e-02 /
CHEB / -1.0723000e-01 -1.0749000e-01 -6.1664000e-03 /

C5H9_1_4+H(+m)=C5H9_2_4+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -2.6496471807607236
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7351000e+00 -1.0606000e+00 -1.2724000e-01 /
CHEB / 3.5286000e+00 1.0397000e+00 3.3282000e-02 /
CHEB / 6.1600000e-01 2.1242000e-01 1.1259000e-01 /
CHEB / -1.2986000e-02 -9.6509000e-02 3.2028000e-02 /
CHEB / -3.9339000e-02 -9.2771000e-02 -2.6504000e-02 /

C5H9_1_4+H(+m)=C3H7-1+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = 1.35024790647401
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0226000e+00 -9.9010000e-01 -1.4622000e-01 /
CHEB / 3.8790000e+00 9.9966000e-01 6.3262000e-02 /
CHEB / 4.9840000e-01 1.6973000e-01 1.1177000e-01 /
CHEB / -4.0379000e-02 -1.0171000e-01 1.9256000e-02 /
CHEB / -4.8457000e-02 -8.2400000e-02 -3.0436000e-02 /

C5H9_1_4+H(+m)=C2H5CHCHCH2+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -15.838369272503193
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2789000e+00 -1.1543000e+00 -1.0929000e-01 /
CHEB / 2.3243000e+00 1.0496000e+00 4.5764000e-03 /
CHEB / 4.6654000e-01 3.0165000e-01 1.0142000e-01 /
CHEB / -3.5147000e-02 -6.3172000e-02 5.2281000e-02 /
CHEB / -5.7691000e-02 -1.0686000e-01 -1.2619000e-02 /

C2H5+aC3H5(+m)=C5H10_1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cs     C_rad/H2/Cd          deltaHrxn(T=298K) = -
76.50215945641996 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2297000e+01 3.9193000e-01 -2.7567000e-02 /
CHEB / -1.4432000e+00 7.1053000e-01 -4.1458000e-02 /
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CHEB / -1.2270000e+00 5.2354000e-01 -9.9779000e-03 /
CHEB / -9.0784000e-01 2.9980000e-01 1.9132000e-02 /
CHEB / -6.2209000e-01 1.1352000e-01 3.1418000e-02 /

C5H9_2_4+H(+m)=C5H10_1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination exact:
C_rad/H/NonDeC     H_rad      deltaHrxn(T=298K) = -98.43953824783776
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2223000e+01 8.3691000e-01 -1.3262000e-01 /
CHEB / -2.4832000e+00 1.2919000e+00 -1.1346000e-01 /
CHEB / -1.7222000e+00 7.2616000e-01 1.8789000e-02 /
CHEB / -1.1224000e+00 2.7692000e-01 6.4239000e-02 /
CHEB / -6.8314000e-01 4.0708000e-02 4.6390000e-02 /

C5H9_2_4+H(+m)=CH3+C4H7-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -9.268992209374126
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0828000e+01 -1.1644000e+00 -1.0052000e-01 /
CHEB / 2.2684000e+00 1.0686000e+00 -4.3905000e-03 /
CHEB / 3.6522000e-01 2.9846000e-01 1.0174000e-01 /
CHEB / -1.1976000e-01 -7.1270000e-02 5.2643000e-02 /
CHEB / -9.6757000e-02 -1.0876000e-01 -1.3799000e-02 /

C5H9_2_4+H(+m)=C2H5+aC3H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -21.937378791417792
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2073000e+01 -1.2252000e+00 -9.1026000e-02 /
CHEB / 1.0031000e+00 1.0535000e+00 -1.8259000e-02 /
CHEB / 8.0829000e-02 3.6318000e-01 8.8648000e-02 /
CHEB / -1.8892000e-01 -3.0286000e-02 6.3206000e-02 /
CHEB / -1.3152000e-01 -1.1130000e-01 1.0015000e-05 /

C5H9_2_4+H(+m)=C2H5CHCHCH2+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -13.18872209174247
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3740000e+00 -1.1949000e+00 -9.5075000e-02 /
CHEB / 2.5126000e+00 1.0640000e+00 -1.1933000e-02 /
CHEB / 4.7193000e-01 3.3065000e-01 9.5449000e-02 /
CHEB / -6.8584000e-02 -5.3727000e-02 5.8325000e-02 /
CHEB / -8.0912000e-02 -1.1166000e-01 -7.4024000e-03 /

C3H7-1+C2H3(+m)=C5H10_1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cs     Cd_pri_rad           deltaHrxn(T=298K) = -
102.4394333350725 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1175000e+01 1.1148000e+00 -2.3202000e-01 /
CHEB / -2.6243000e+00 1.4516000e+00 -1.0053000e-01 /
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CHEB / -1.8522000e+00 7.3940000e-01 4.7046000e-02 /
CHEB / -1.1474000e+00 2.4721000e-01 7.5127000e-02 /
CHEB / -6.7987000e-01 2.1403000e-02 4.3120000e-02 /

C3H7-1+C2H3(+m)=CH3+C4H7-14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -13.26888729660886
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0575000e+01 -1.0689000e+00 -1.3321000e-01 /
CHEB / 1.8488000e+00 1.0199000e+00 3.8263000e-02 /
CHEB / 3.2318000e-01 2.3963000e-01 1.0839000e-01 /
CHEB / -7.2195000e-02 -8.4111000e-02 3.7145000e-02 /
CHEB / -7.0859000e-02 -9.6433000e-02 -2.2662000e-02 /

C3H7-1+C2H3(+m)=C2H5+aC3H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -25.937273878652526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1617000e+01 -1.1149000e+00 -1.3104000e-01 /
CHEB / 7.7705000e-01 1.0098000e+00 2.7918000e-02 /
CHEB / 2.6454000e-02 2.9148000e-01 1.0371000e-01 /
CHEB / -1.4724000e-01 -5.5467000e-02 4.8800000e-02 /
CHEB / -1.0146000e-01 -1.0098000e-01 -1.3384000e-02 /

C3H7-1+C2H3(+m)=C5H9_2_4+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -3.9998950872347336
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6405000e+00 -1.0132000e+00 -1.4154000e-01 /
CHEB / 3.2220000e+00 1.0099000e+00 5.4909000e-02 /
CHEB / 5.9649000e-01 1.8708000e-01 1.1172000e-01 /
CHEB / -3.0214000e-04 -9.9309000e-02 2.4111000e-02 /
CHEB / -3.7444000e-02 -8.6345000e-02 -2.9018000e-02 /

C3H7-1+C2H3(+m)=C2H5CHCHCH2+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -17.188617178977204
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0214000e+00 -1.0922000e+00 -1.3141000e-01 /
CHEB / 2.1934000e+00 1.0171000e+00 3.2683000e-02 /
CHEB / 4.1944000e-01 2.6530000e-01 1.0609000e-01 /
CHEB / -2.3556000e-02 -7.1785000e-02 4.2939000e-02 /
CHEB / -5.2774000e-02 -9.9654000e-02 -1.8467000e-02 /

C2H5CHCHCH2+H(+m)=C5H10_1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
85.25081615609528 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2970000e+01 4.9070000e-01 -4.3673000e-02 /
CHEB / -1.8169000e+00 8.7113000e-01 -6.2522000e-02 /
CHEB / -1.3803000e+00 6.0391000e-01 -1.0394000e-02 /
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CHEB / -9.8373000e-01 3.1063000e-01 2.9968000e-02 /
CHEB / -6.4189000e-01 9.4074000e-02 3.9452000e-02 /

C2H5CHCHCH2+H(+m)=CH3+C4H7-14(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = 3.919729882368351
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1804000e+00 -1.2904000e+00 -6.5930000e-02 /
CHEB / 4.5129000e+00 1.0636000e+00 -3.8991000e-02 /
CHEB / 3.2397000e-01 4.1804000e-01 6.9960000e-02 /
CHEB / -1.9366000e-01 -7.5287000e-03 6.8822000e-02 /
CHEB / -1.2927000e-01 -1.1853000e-01 1.0715000e-02 /

C2H5CHCHCH2+H(+m)=C2H5+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #18 (C5H10_1)     deltaHrxn(T=298K) = -8.748656699675315
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1169000e+01 -1.3673000e+00 -5.0700000e-02 /
CHEB / 2.4022000e+00 1.0168000e+00 -4.6189000e-02 /
CHEB / 2.3712000e-01 4.9422000e-01 4.2295000e-02 /
CHEB / -2.7138000e-01 6.9707000e-02 6.6168000e-02 /
CHEB / -1.8346000e-01 -1.0159000e-01 2.8724000e-02 /

!PDepNetwork nSPC(1064)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(1064)        -32.18      82.09 18.6  23.76 26.63 28.84 32.15
      34.51 36.15 null
!     nSPC(102)         51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57
      23.05 null
!     CO2               -94.36      50.99 8.87  9.84  10.63 11.26 12.23
      12.9  13.82
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(102)+CO2=nSPC(1064)      1.9263655e+11      0.04067
9.2900000e+03

nSPC(1064)(+m)=nSPC(102)+CO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (nSPC(1064))   deltaHrxn(T=298K) = -11.069452833026304
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0445000e+00 2.0000000e+00 -1.3651000e-05 /
CHEB / 8.3477000e-01 -2.0826000e-05 -1.4495000e-05 /
CHEB / -1.4061000e+00 -6.0454000e-06 -4.2068000e-06 /
CHEB / -6.1502000e-01 -1.2450000e-06 -8.6589000e-07 /
CHEB / -2.5066000e-01 -3.3209000e-07 -2.3076000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
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!Here are the species and their thermochemistry:
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     CH2CO             -10.78      57.63 12.31 14.11 15.57 16.77 18.67
      20.12 22.44
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+CO=unknown1(2)           2.3501400e+11      0.30815
4.9629937e+03
!     O+CH2CO=unknown1(2)     2.3501400e+11      0.30815
4.9629937e+03

O+CH2CO(+m)=CH2O+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#11 (unknown1)    deltaHrxn(T=298K) = -101.509551858014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0435000e+01 1.2812000e-15 -1.0902000e-15 /
CHEB / 1.6253000e+00 -2.4893000e-15 2.1180000e-15 /
CHEB / 2.2256000e-02 2.2816000e-15 -1.9403000e-15 /
CHEB / 1.6951000e-02 -1.9655000e-15 1.6727000e-15 /
CHEB / -2.0641000e-03 1.5845000e-15 -1.3479000e-15 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     sSPC(1697)        3.82  64.41 12.08 14.18 16.24 18.05 20.9  23.01
      26.26
!     CH2CO             -10.78      57.63 12.31 14.11 15.57 16.77 18.67
      20.12 22.44
!     HO2         3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26 12.25
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+O2=nSPC(543)     2.2600000e+12      0.00000
0.0000000e+00
!     CO+sSPC(1697)=nSPC(543)       9.1400000e+04      2.53000
8.5500000e+04
!     nSPC(543)=CH2CO+HO2     5.8013126e+10      0.62333
3.0055556e+04

nSPC(543)(+m)=CO+sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543))    deltaHrxn(T=298K) = -4.529477583957297
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1756000e+01 4.6250000e+00 9.5865000e-01 /
CHEB / 2.5845000e+01 6.8980000e-01 1.6630000e-01 /
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CHEB / -1.2952000e+00 1.5503000e-01 3.1518000e-02 /
CHEB / -6.4343000e-01 2.3582000e-02 1.2262000e-03 /
CHEB / -2.8348000e-01 -7.8498000e-03 -5.5593000e-03 /

!CH2CHO+O2(+m)=nSPC(543)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/CO     O2_birad       deltaHrxn(T=298K) = -
23.517625019811888 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 1.0045000e+01 1.4755000e+00 -1.8876000e-01 /
!CHEB / -2.4528000e+00 4.4674000e-01 1.6691000e-01 /
!CHEB / -1.4152000e+00 1.2913000e-01 4.2330000e-02 /
!CHEB / -6.8852000e-01 -1.1263000e-02 -4.6142000e-03 /
!CHEB / -3.0430000e-01 -3.1781000e-02 -1.1111000e-02 /

CH2CHO+O2(+m)=CO+sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543))    deltaHrxn(T=298K) = -28.047102603769186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0979000e+01 1.0478000e-06 7.2935000e-07 /
CHEB / 2.0343000e+01 1.6351000e-06 1.1381000e-06 /
CHEB / 1.4894000e-01 9.2011000e-07 6.4047000e-07 /
CHEB / 3.0755000e-02 3.3879000e-07 2.3582000e-07 /
CHEB / -5.4325000e-03 -3.3615000e-09 -2.3396000e-09 /

!CH2CHO+O2(+m)=CH2CO+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543))    deltaHrxn(T=298K) = -13.138807536396591
kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 7.8898000e+00 -4.5991000e-02 -3.3898000e-02 /
!CHEB / 3.0748000e+00 5.4169000e-02 3.9917000e-02 /
!CHEB / 2.5318000e-01 1.0042000e-04 -2.8720000e-05 /
!CHEB / 7.6717000e-02 -8.4981000e-03 -6.0804000e-03 /
!CHEB / 2.1522000e-02 -1.5827000e-03 -1.1797000e-03 /

!CH2CO+HO2(+m)=nSPC(543)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543))    deltaHrxn(T=298K) = -10.3788174834153
kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / -2.7614000e+00 2.9906000e+00 5.6272000e-02 /
!CHEB / 5.1642000e+00 2.2780000e-01 -4.6751000e-03 /
!CHEB / -1.0963000e+00 4.8689000e-02 7.2809000e-03 /
!CHEB / -5.5135000e-01 -2.2831000e-02 -1.0489000e-02 /
!CHEB / -2.4509000e-01 -3.1208000e-02 -1.2073000e-02 /

CH2CO+HO2(+m)=CO+sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(543))    deltaHrxn(T=298K) = -14.908295067372597
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9620000e+01 -2.2551000e-05 -1.5699000e-05 /
CHEB / 2.5991000e+01 1.1637000e-05 8.1013000e-06 /
CHEB / 5.0960000e-01 1.0228000e-05 7.1206000e-06 /
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CHEB / 1.7498000e-01 3.1778000e-06 2.2122000e-06 /
CHEB / 5.3272000e-02 1.2411000e-08 8.5042000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     CH3CO             -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81
      26.16
!     CH2CO             -10.78      57.63 12.31 14.11 15.57 16.77 18.67
      20.12 22.44
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+H=CH2CHO          3.4049294e+12      0.23000
3.1333333e+03
!     CH2CHO=CH3CO                  2.0320555e+08      1.13906
3.4790987e+04
!     CH2CO+H=CH3CO           1.8833259e+13      0.00000
2.9000000e+03
!     CH3+CO=CH3CO            5.0600000e+11      0.00000
6.8800000e+03

CH3+CO(+m)=CH2CHO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (CH2CHO) deltaHrxn(T=298K) = -4.059003964843025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1892000e+00 6.6886000e-01 -1.1232000e-01 /
CHEB / 9.6907000e+00 8.5108000e-01 -3.6307000e-02 /
CHEB / -6.6794000e-01 3.1724000e-01 5.6658000e-02 /
CHEB / -3.8304000e-01 5.0251000e-02 3.9524000e-02 /
CHEB / -1.9588000e-01 -2.3609000e-02 7.5850000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     CH2CO             -10.78      57.63 12.31 14.11 15.57 16.77 18.67
      20.12 22.44
!     HO2         3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26 12.25
!     sSPC(1909)        -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45
      25.52 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
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!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+HO2=nSPC(801)     2.7411173e+10      0.56667
3.7888889e+03
!     sSPC(1909)+OH=nSPC(801) 2.0000000e+13      0.00000
0.0000000e+00
!     CH3CO+O2=unknown1(2)    1.5050000e+12      0.00000
0.0000000e+00
!     unknown1(2)=CH2CO+HO2   4.3669559e+09      1.31333
2.9866667e+04

CH2CO+HO2(+m)=nSPC(801)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Cd/H2     O_rad/NonDe         deltaHrxn(T=298K)
= -26.95731013924095 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0225000e+00 1.5126000e+00 -7.3651000e-04 /
CHEB / -7.2582000e-01 3.6691000e-01 -5.6152000e-02 /
CHEB / -1.2290000e+00 1.2904000e-01 5.9504000e-02 /
CHEB / -5.8905000e-01 2.7484000e-02 4.8356000e-03 /
CHEB / -2.7416000e-01 -2.1299000e-02 -2.9803000e-03 /

sSPC(1909)+OH(+m)=nSPC(801)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     O_pri_rad      deltaHrxn(T=298K) = -
40.975780301620645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1687000e+00 3.6523000e+00 1.7699000e-01 /
CHEB / -1.4032000e+00 2.3245000e-01 -6.0696000e-03 /
CHEB / -1.0492000e+00 -6.3266000e-02 -4.3231000e-03 /
CHEB / -5.6205000e-01 2.4714000e-02 -2.6887000e-02 /
CHEB / -3.0763000e-01 6.9897000e-02 -4.1093000e-02 /

sSPC(1909)+OH(+m)=CH2CO+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801))    deltaHrxn(T=298K) = -14.0184701623797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3478000e+01 -7.2772000e-05 -6.6169000e-05 /
CHEB / -2.0150000e-01 2.7629000e-05 2.3856000e-05 /
CHEB / -3.0953000e-02 8.6994000e-05 7.5371000e-05 /
CHEB / 1.6322000e-02 7.2907000e-07 2.5243000e-06 /
CHEB / 7.6536000e-03 -3.6239000e-05 -2.9581000e-05 /

sSPC(1909)+OH(+m)=CH3CO+O2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801))    deltaHrxn(T=298K) = -7.578918522238124
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0263000e+01 -1.0489000e-01 -7.0728000e-02 /
CHEB / 3.2722000e-02 1.1342000e-01 7.6650000e-02 /
CHEB / -1.8943000e-01 1.4371000e-02 8.8409000e-03 /
CHEB / -9.0394000e-02 -2.0080000e-02 -1.2509000e-02 /
CHEB / -3.3910000e-02 -7.0332000e-03 -4.7639000e-03 /
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CH3CO+O2(+m)=nSPC(801)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801))    deltaHrxn(T=298K) = -33.396861779382526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5449000e+00 7.3631000e-01 -3.2741000e-01 /
CHEB / -2.5418000e+00 1.5732000e+00 1.5620000e-01 /
CHEB / -1.6031000e+00 3.7310000e-01 1.0862000e-01 /
CHEB / -8.0785000e-01 -6.4090000e-02 3.2521000e-02 /
CHEB / -3.6557000e-01 -1.0854000e-01 -1.0438000e-02 /

CH3CO+O2(+m)=CH2CO+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (nSPC(801))    deltaHrxn(T=298K) = -6.439551640141575
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1488000e+01 -5.6000000e-01 -1.8773000e-01 /
CHEB / 6.9620000e-01 6.4531000e-01 1.9112000e-01 /
CHEB / 6.6863000e-03 1.4035000e-02 3.4459000e-02 /
CHEB / -3.2126000e-02 -9.0689000e-02 -2.1848000e-02 /
CHEB / -1.0774000e-02 -2.7278000e-02 -1.9501000e-02 /

!PDepNetwork nSPC(879)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!     nSPC(1064)        -32.18      82.09 18.6  23.76 26.63 28.84 32.15
      34.51 36.15 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(801)+O2=nSPC(879)  2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(1064)+OH=nSPC(879) 2.0000000e+13      0.00000
0.0000000e+00

nSPC(801)+O2(+m)=nSPC(879)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(879)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/CO     O2_birad       deltaHrxn(T=298K) = -
31.506271526489577 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0868000e+01 6.6223000e-01 -5.3277000e-02 /
CHEB / -2.9136000e+00 1.0218000e+00 -3.5030000e-02 /
CHEB / -2.0344000e+00 4.5618000e-01 4.8670000e-02 /
CHEB / -1.2129000e+00 4.4249000e-02 5.1411000e-02 /
CHEB / -6.0906000e-01 -1.1087000e-01 9.2673000e-03 /

nSPC(1064)+OH(+m)=nSPC(879)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(879)) High-P Limit: R_Recombination estimate:
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(Average:) O_rad/OneDe     O_pri_rad      deltaHrxn(T=298K) = -
42.00558613338494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0539000e+01 1.9329000e+00 -4.5327000e-01 /
CHEB / -3.8002000e+00 1.5067000e+00 8.5484000e-02 /
CHEB / -2.3586000e+00 4.1083000e-01 1.3950000e-01 /
CHEB / -1.2673000e+00 -4.1726000e-02 5.4780000e-02 /
CHEB / -6.0406000e-01 -1.3625000e-01 -6.7079000e-03 /

nSPC(1064)+OH(+m)=nSPC(801)+O2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (nSPC(879))    deltaHrxn(T=298K) = -10.499314606895364
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2650000e+01 -7.3240000e-01 -1.9476000e-01 /
CHEB / 4.1783000e-01 8.0760000e-01 1.6212000e-01 /
CHEB / -9.3959000e-02 5.5183000e-02 8.0247000e-02 /
CHEB / -8.6029000e-02 -9.7740000e-02 -1.6002000e-02 /
CHEB / -2.2678000e-02 -4.7628000e-02 -2.9570000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown(1)        -6.28 104.42      32.13 36.66 39.96 42.72 46.81
      50.04 51.65 null
!     nSPC(1064)        -32.18      82.09 18.6  23.76 26.63 28.84 32.15
      34.51 36.15 null
!     HO2         3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26 12.25
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(1064)+HO2=unknown(1)     2.7411173e+10      0.56667
3.7888889e+03
!     nSPC(879)+O=unknown(1)        2.3501400e+11      0.30815
4.9629937e+03

nSPC(879)+O(+m)=nSPC(1064)+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown)      deltaHrxn(T=298K) = -23.247294898888057
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9833000e+00 2.9004000e-12 2.0171000e-12 /
CHEB / 2.2520000e+00 1.2151000e-11 8.4617000e-12 /
CHEB / -2.2856000e-01 2.5162000e-11 1.7512000e-11 /
CHEB / 1.9740000e-02 3.2531000e-11 2.2647000e-11 /
CHEB / 7.0423000e-03 2.7240000e-11 1.8958000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     unknown1(1)       -72.28      74.14 14.28 19.11 22.17 24.71 28.83
      31.46 34.04 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     OH+CH2CHO=unknown1(1)         1.4157154e+13      -0.15000
2.9166667e+02
!     CH2OH+HCO=unknown1(1)         1.4157154e+13      -0.15000
2.9166667e+02
!     CH3OH+CO=unknown1(1)          9.1400000e+04      2.53000
8.5500000e+04

OH+CH2CHO(+m)=CH2OH+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -7.199307154055264
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2121000e+01 -5.0306000e-01 -1.9929000e-01 /
CHEB / 3.2632000e-01 5.6193000e-01 1.9819000e-01 /
CHEB / 1.3842000e-02 2.6832000e-02 4.0161000e-02 /
CHEB / -1.7432000e-02 -7.1372000e-02 -2.3172000e-02 /
CHEB / -1.6684000e-02 -2.6664000e-02 -1.8674000e-02 /

OH+CH2CHO(+m)=CH3OH+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -88.34083960870265
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0461000e+00 -4.8770000e-01 -1.8841000e-01 /
CHEB / 1.6642000e+00 5.6086000e-01 1.9184000e-01 /
CHEB / 3.5501000e-01 3.7503000e-03 3.3506000e-02 /
CHEB / 8.1460000e-02 -6.8671000e-02 -2.4106000e-02 /
CHEB / 2.0798000e-02 -1.9955000e-02 -1.6409000e-02 /

CH2OH+HCO(+m)=CH3OH+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -81.14153245464739
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0072000e+00 -6.2969000e-01 -1.9664000e-01 /
CHEB / 2.7851000e+00 7.1024000e-01 1.7953000e-01 /
CHEB / 2.8333000e-01 2.0898000e-02 6.0255000e-02 /
CHEB / 6.4878000e-02 -8.4588000e-02 -2.1589000e-02 /
CHEB / 1.5053000e-02 -3.0364000e-02 -2.3455000e-02 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -92.0 76.36 18.58 22.7  26.24 29.32 34.26 37.88
      39.54 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!Here are the path reactions and their high-P limit kinetics:
!     OH+C2H5O-1=unknown2(2)        7.7000000e+13      0.00000
0.0000000e+00
!     CH2OH+CH2OH=unknown2(2)       1.1500000e+13      0.00000
0.0000000e+00
!     C2H4O+H2O=unknown2(2)         2.2700000e+02      2.74000
5.6900000e+04

OH+C2H5O-1(+m)=CH2OH+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown2)     deltaHrxn(T=298K) = -10.578772430778123
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3549000e+01 -6.5302000e-01 -2.0749000e-01 /
CHEB / 3.3983000e-01 7.0388000e-01 1.8584000e-01 /
CHEB / -2.5032000e-02 6.1948000e-02 6.3655000e-02 /
CHEB / -7.7304000e-02 -8.2312000e-02 -1.7155000e-02 /
CHEB / -5.0240000e-02 -4.1180000e-02 -2.3478000e-02 /

OH+C2H5O-1(+m)=C2H4O+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown2)     deltaHrxn(T=298K) = -90.47073366481744
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1706000e+01 -6.3390000e-01 -2.4887000e-01 /
CHEB / 6.6657000e-01 6.4558000e-01 2.0738000e-01 /
CHEB / -9.5206000e-02 1.0014000e-01 8.4106000e-02 /
CHEB / -1.1429000e-01 -6.0322000e-02 -5.5562000e-03 /
CHEB / -6.8449000e-02 -4.8909000e-02 -2.5136000e-02 /

CH2OH+CH2OH(+m)=C2H4O+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown2)     deltaHrxn(T=298K) = -79.89196123403931
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0873000e+01 -1.2713000e+00 -7.5658000e-02 /
CHEB / 1.0334000e+00 1.0399000e+00 -3.2994000e-02 /
CHEB / -1.1851000e-01 3.8732000e-01 6.9116000e-02 /
CHEB / -2.0094000e-01 1.0010000e-03 6.0591000e-02 /
CHEB / -1.1678000e-01 -9.2026000e-02 1.2539000e-02 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -65.8 74.24 19.09 23.18 26.8  29.85 34.57 37.97
      37.97 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!Here are the path reactions and their high-P limit kinetics:
!     HCO+CH2CHO=unknown3(3)        1.4157154e+13      -0.15000
2.9166667e+02
!     CO+CH3CHO=unknown3(3)         9.1400000e+04      2.53000
8.5500000e+04

HCO+CH2CHO(+m)=CO+CH3CHO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (unknown3)     deltaHrxn(T=298K) = -80.50177340482311
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1660000e+00 -8.2797000e-01 -1.7078000e-01 /
CHEB / 3.2859000e+00 8.4567000e-01 1.2130000e-01 /
CHEB / 2.1582000e-01 1.0968000e-01 7.5755000e-02 /
CHEB / -3.4365000e-02 -7.6758000e-02 1.9442000e-03 /
CHEB / -4.4809000e-02 -4.9114000e-02 -1.8994000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H5OJ(13)        7.36  75.41 19.41 22.49 25.45 28.06 32.31 35.53
      40.59
!     C3H5OJ(12)        -4.96 71.27 18.06 21.58 24.93 27.85 32.53 36.02
      41.39
!     C3H5OJ(8)         -6.18 74.68 17.76 20.93 24.04 26.82 31.36 34.8
      40.18
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C3H5OJ      27.09 76.26 18.34 21.54 24.52 27.2  31.62 34.9  39.89
      null
!     CH2CHCH2O         25.06 72.63 18.45 22.37 25.85 28.76 33.26 36.56
      41.63
!     CHCHCH2OH         29.29 75.84 18.49 22.0  25.1  27.8  32.14 35.32
      40.12 null
!     C3H5OJ(17)        22.25 72.17 19.21 23.32 26.93 29.77 33.8  36.58
      40.96  !MRH CBS-QB3 w/1DHR corrections
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!     CH3CHcOH          21.62 72.89 19.21 23.08 26.31 28.95 32.97 35.9
      40.57 null
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C3H4O-enone             -13.82      68.58 16.45 19.54 22.36 24.81
      28.75 31.71 36.31
!     C3H3OH            4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94
      36.79 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     CH2O        -26.22      52.16 8.44  9.33  10.38 11.42 13.25 14.69
      16.9
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+HCO=C3H5OJ(13)     5.2000000e+11      0.00000
6.5600000e+03
!     C3H4O+H=C3H5OJ(13)      2.8500000e+13      0.00000
4.3000000e+03
!     C2H5+CO=C3H5OJ(13)      4.0416992e+07      1.70125
8.2775000e+04
!     C3H5OJ(13)=C3H5OJ(12)         5.6400000e+08      1.28000
2.7900000e+04
!     C3H4O+H=C3H5OJ(12)      3.7100000e+13      0.00000
1.0000000e+03
!     C3H4O-enone+H=C3H5OJ(12)      3.4049294e+12      0.23000
3.1333333e+03
!     C3H5OJ(12)=C3H5OJ(8)          2.0320555e+08      1.13906
3.4790987e+04
!     C3H5OJ(12)=C3H5O-enol2        3.5266395e+10      0.61833
2.7168333e+04
!     C3H3OH+H=C3H5O-enol2    1.2800000e+13      0.00000
3.7000000e+03
!     C3H4O+H=C3H5O-enol2     2.3501400e+11      0.30815
4.9629937e+03
!     C3H5OJ=C3H5O-enol2            2.8960000e+10      0.82000
3.7500000e+04
!     CH2CHCH2O=C3H5O-enol2         8.1282219e+08      1.13906
3.4790987e+04
!     C2H3+CH2O=CH2CHCH2O     3.2847733e+07      1.50370
7.3354000e+03
!     C3H4O+H=CH2CHCH2O       1.0000000e+11      0.00000
1.1900000e+04
!     CH2CHCH2O=CHCHCH2OH           8.1282219e+08      1.13906
3.4790987e+04
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```
!     CH2CHCH2O=C3H5OJ              2.0320555e+08      1.13906
3.4790987e+04
!     aC3H5+O=CH2CHCH2O       1.0000000e+13      0.00000
0.0000000e+00
!     CHCHCH2OH=C3H5O-enol2         3.6920000e+10      0.74000
3.4700000e+04
!     C3H5OJ(17)=C3H5O-enol2        2.1960000e+10      1.12000
4.1300000e+04
!     CH3CHcOH=C3H5O-enol2          2.3220000e+10      1.08000
3.8700000e+04
!     C3H5OJ(12)=CH3CHcOH           2.0320555e+08      1.13906
3.4790987e+04
!     C3H5OJ(12)=C3H5OJ(17)         2.0320555e+08      1.13906
3.4790987e+04
!     pC3H5+O=C3H5OJ(12)      1.0000000e+13      0.00000
0.0000000e+00
!     C3H5OJ(13)=C3H5OJ(8)          2.0320555e+08      1.13906
3.4790987e+04

C3H5OJ(13)(+m)=C3H5OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -12.318543415985497 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7696000e+00 2.6823000e+00 -3.7795000e-01 /
CHEB / 6.9067000e+00 6.6488000e-01 5.1622000e-03 /
CHEB / -1.9385000e+00 2.4908000e-01 3.2516000e-03 /
CHEB / -1.1264000e+00 -2.2229000e-02 -1.2097000e-02 /
CHEB / -5.8486000e-01 -1.0979000e-01 -1.4851000e-02 /

C3H5OJ(13)(+m)=C3H5O-enol2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -8.738939485679419
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6951000e+00 2.1996000e+00 -6.0607000e-01 /
CHEB / 7.1136000e+00 1.2427000e+00 2.2173000e-01 /
CHEB / -2.0505000e+00 2.7217000e-01 6.0502000e-02 /
CHEB / -1.2192000e+00 -1.0671000e-01 -3.3022000e-02 /
CHEB / -6.1926000e-01 -1.5929000e-01 -4.0672000e-02 /

C3H5OJ(13)(+m)=C2H5+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -4.369524279882775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6234000e+01 1.1643000e+01 -2.2509000e-01 /
CHEB / 2.4240000e+01 -3.9703000e-01 1.2062000e+00 /
CHEB / -1.4889000e+00 -9.8596000e-01 1.5821000e-01 /
CHEB / -7.0026000e-01 -6.0032000e-01 -2.7403000e-02 /
CHEB / -3.5702000e-01 -2.3830000e-01 3.6586000e-02 /

C3H5O-enol2(+m)=C3H5OJ(12)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -3.579603930306077
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.2132000e+00 7.9272000e-01 -9.3819000e-02 /
CHEB / 5.0757000e+00 1.0195000e+00 -4.5785000e-03 /
CHEB / -1.9881000e+00 3.2351000e-01 7.6629000e-02 /
CHEB / -1.1547000e+00 -5.3940000e-02 3.7089000e-02 /
CHEB / -5.9283000e-01 -1.4681000e-01 -1.4942000e-02 /

C3H5O-enol2(+m)=C2H5+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 4.369415205796642
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5831000e+01 1.1363000e+01 -7.5568000e-01 /
CHEB / 2.5279000e+01 -3.7020000e-01 1.3974000e+00 /
CHEB / -1.9634000e+00 -1.1933000e+00 4.6565000e-01 /
CHEB / -9.4424000e-01 -5.6504000e-01 4.4444000e-02 /
CHEB / -5.8258000e-01 -2.6601000e-02 -8.9938000e-02 /

CH2CHCH2O(+m)=C3H5OJ(13)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -17.698403883846524
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3951000e+01 8.0992000e+00 -1.3918000e+00 /
CHEB / 8.0409000e+00 1.5048000e+00 8.2293000e-01 /
CHEB / -2.4290000e+00 -2.3611000e-01 3.9786000e-01 /
CHEB / -1.2239000e+00 -3.7984000e-01 8.9201000e-02 /
CHEB / -5.5899000e-01 -2.0460000e-01 -3.0660000e-02 /

CH2CHCH2O(+m)=C3H5OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -30.01694729983202
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0260000e+01 7.0574000e+00 -1.4303000e+00 /
CHEB / 6.3622000e+00 1.8220000e+00 8.1830000e-01 /
CHEB / -2.8963000e+00 3.0075000e-02 3.5895000e-01 /
CHEB / -1.4405000e+00 -2.1432000e-01 6.9397000e-02 /
CHEB / -6.9099000e-01 -1.2277000e-01 -3.9799000e-02 /

CH2CHCH2O(+m)=C3H5O-enol2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    O_rad_out     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -26.43734336952594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0697000e+01 7.3406000e+00 -1.3089000e+00 /
CHEB / 6.0360000e+00 1.5820000e+00 6.9517000e-01 /
CHEB / -3.0234000e+00 7.7885000e-03 3.5948000e-01 /
CHEB / -1.4860000e+00 -2.2647000e-01 7.6157000e-02 /
CHEB / -7.0261000e-01 -1.3262000e-01 -4.1727000e-02 /

CH2CHCH2O(+m)=C2H4+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -1.4298798090239622
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -6.8784000e+00 2.1566000e+00 -5.7578000e-01 /
CHEB / 9.3648000e+00 1.0870000e+00 5.6526000e-01 /
CHEB / -1.8612000e+00 5.5034000e-02 8.4604000e-02 /
CHEB / -9.9064000e-01 -1.1185000e-01 -3.4593000e-02 /
CHEB / -4.4535000e-01 -7.2096000e-02 -3.0464000e-02 /

CH2CHCH2O(+m)=C2H5+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -22.0679281637293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8985000e+01 8.7508000e+00 7.9853000e-02 /
CHEB / 1.8708000e+01 -1.6219000e+00 9.4118000e-01 /
CHEB / -1.2004000e+00 -1.2768000e+00 1.3070000e-01 /
CHEB / -6.7252000e-01 -5.0493000e-01 -2.7703000e-02 /
CHEB / -4.1536000e-01 -5.3424000e-02 -1.0952000e-02 /

C2H4+HCO(+m)=C3H5OJ(13)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H2     CO_pri_rad       deltaHrxn(T=298K)
= -16.26852407482256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0994000e+00 1.2427000e+00 -2.0271000e-01 /
CHEB / -8.0307000e-02 6.0471000e-01 1.6251000e-01 /
CHEB / -1.4533000e+00 2.0531000e-01 5.5012000e-02 /
CHEB / -7.6212000e-01 -1.5059000e-02 2.5411000e-03 /
CHEB / -3.5960000e-01 -5.8310000e-02 -1.2882000e-02 /

C2H4+HCO(+m)=C3H5OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -28.587067490808057
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2643000e+00 5.4918000e-01 -2.3198000e-01 /
CHEB / 2.9840000e+00 1.3813000e+00 2.0201000e-02 /
CHEB / -1.2776000e+00 5.7757000e-01 2.0048000e-02 /
CHEB / -9.0145000e-01 1.0531000e-01 3.6217000e-02 /
CHEB / -5.1101000e-01 -6.3165000e-02 1.8272000e-02 /

C2H4+HCO(+m)=C3H5O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -25.00746356050198
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3905000e+00 1.3978000e-01 -4.4040000e-01 /
CHEB / 3.1749000e+00 1.9434000e+00 2.4456000e-01 /
CHEB / -1.4290000e+00 5.4227000e-01 5.9069000e-02 /
CHEB / -1.0003000e+00 7.1596000e-03 2.8983000e-03 /
CHEB / -5.3638000e-01 -1.0067000e-01 -7.0358000e-03 /

C2H4+HCO(+m)=C2H5+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -20.638048354705337
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2983000e+01 5.6089000e-06 2.0869000e-06 /
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CHEB / 2.1677000e+01 2.7863000e-05 2.0433000e-05 /
CHEB / 1.1194000e-01 9.1489000e-06 8.1402000e-06 /
CHEB / 7.5775000e-03 -1.2130000e-05 -8.8673000e-06 /
CHEB / -1.6865000e-02 -1.3631000e-05 -1.0378000e-05 /

C3H4O+H(+m)=C3H5OJ(13)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/De_Cd/H2     H_rad       deltaHrxn(T=298K) = -30.536590361845093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2026000e+00 2.3910000e+00 1.4351000e-02 /
CHEB / -8.1681000e-01 8.9742000e-01 -2.8809000e-01 /
CHEB / -1.3725000e+00 2.7330000e-01 -1.8933000e-02 /
CHEB / -7.7774000e-01 4.9339000e-02 6.8584000e-02 /
CHEB / -3.8460000e-01 -6.2959000e-02 3.5630000e-02 /

C3H4O+H(+m)=C3H5OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H/De     H_rad       deltaHrxn(T=298K) = -42.85513377783059
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1730000e+01 1.0125000e+00 -1.5652000e-01 /
CHEB / -2.3093000e+00 1.3730000e+00 -1.5584000e-01 /
CHEB / -1.7087000e+00 6.3111000e-01 2.7098000e-02 /
CHEB / -9.8373000e-01 1.5111000e-01 6.5848000e-02 /
CHEB / -5.1936000e-01 -4.2822000e-02 2.6943000e-02 /

C3H4O+H(+m)=C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
39.27552984752451 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0901000e+01 6.5313000e-01 -3.7496000e-01 /
CHEB / -2.1764000e+00 1.8717000e+00 8.2737000e-02 /
CHEB / -1.8477000e+00 6.0914000e-01 6.5691000e-02 /
CHEB / -1.0791000e+00 5.6018000e-02 2.9513000e-02 /
CHEB / -5.4706000e-01 -8.3364000e-02 1.7936000e-04 /

C3H4O+H(+m)=CH2CHCH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H/De_O     H_rad        deltaHrxn(T=298K) = -
12.838186477998569 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7515000e+00 4.2452000e-01 3.5394000e-02 /
CHEB / 1.3395000e+00 6.1566000e-01 7.0715000e-02 /
CHEB / -1.7354000e+00 2.1930000e-01 4.5445000e-02 /
CHEB / -9.3165000e-01 -9.0498000e-03 8.0946000e-03 /
CHEB / -4.2409000e-01 -5.4797000e-02 -1.0947000e-02 /

C3H4O+H(+m)=C2H4+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -14.268066287022533
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.2147000e+01 -5.3004000e-01 6.1570000e-02 /
CHEB / 1.3705000e+00 4.8735000e-01 -1.3324000e-01 /
CHEB / -5.2016000e-02 1.1918000e-01 4.7143000e-02 /
CHEB / -8.0638000e-02 -7.8853000e-03 4.8502000e-02 /
CHEB / -4.8680000e-02 -4.7731000e-02 3.6790000e-03 /

C3H4O+H(+m)=C2H5+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -34.90611464172787 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5393000e+00 -7.6860000e-03 -6.2568000e-03 /
CHEB / 1.7585000e+01 1.0035000e-02 8.1185000e-03 /
CHEB / 2.2809000e-01 -1.4309000e-03 -1.0304000e-03 /
CHEB / 5.8669000e-02 -1.4314000e-03 -1.2656000e-03 /
CHEB / 1.0836000e-02 2.3988000e-04 1.8760000e-04 /

C3H4O+H(+m)=C3H4O-enone+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 0.38001121023250306
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0914000e+01 -9.6683000e-01 -1.1779000e-01 /
CHEB / 2.1615000e+00 9.9151000e-01 3.5861000e-02 /
CHEB / 4.6191000e-02 1.4846000e-01 1.0535000e-01 /
CHEB / -4.8484000e-02 -1.0406000e-01 2.2997000e-02 /
CHEB / 1.7789000e-04 -7.4261000e-02 -2.8040000e-02 /

C2H5+CO(+m)=C3H5OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -7.949019136102721
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6572000e+01 1.1197000e+01 -7.9012000e-01 /
CHEB / 2.4793000e+01 -2.8686000e-01 1.4073000e+00 /
CHEB / -1.5176000e+00 -1.1390000e+00 4.8418000e-01 /
CHEB / -7.7649000e-01 -5.4292000e-01 4.6819000e-02 /
CHEB / -5.3000000e-01 -1.7460000e-02 -8.7863000e-02 /

C3H4O-enone+H(+m)=C3H5OJ(13)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -30.916601572077596
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4637000e+00 2.2308000e+00 -3.1159000e-01 /
CHEB / -1.1584000e-01 1.4599000e+00 -8.9273000e-02 /
CHEB / -1.3461000e+00 4.3136000e-01 9.6689000e-02 /
CHEB / -8.2107000e-01 -3.2171000e-02 7.0234000e-02 /
CHEB / -4.1394000e-01 -1.2300000e-01 1.4307000e-02 /

C3H4O-enone+H(+m)=C3H5OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Cd/H/Nd     H_rad       deltaHrxn(T=298K) = -
43.23514498806309 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0243000e+01 1.3015000e+00 -2.4960000e-01 /
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CHEB / -1.8366000e+00 1.6043000e+00 -1.7563000e-01 /
CHEB / -1.7936000e+00 6.4714000e-01 6.3093000e-02 /
CHEB / -1.0015000e+00 1.2333000e-01 8.1119000e-02 /
CHEB / -5.2254000e-01 -5.8691000e-02 2.6693000e-02 /

C3H4O-enone+H(+m)=C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -39.65554105775701
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4691000e+00 1.0193000e+00 -4.5072000e-01 /
CHEB / -1.7626000e+00 2.0257000e+00 5.5192000e-02 /
CHEB / -1.9375000e+00 6.1167000e-01 8.7701000e-02 /
CHEB / -1.0911000e+00 3.6221000e-02 4.4820000e-02 /
CHEB / -5.4648000e-01 -9.2541000e-02 3.5167000e-03 /

C3H4O-enone+H(+m)=CH2CHCH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -13.218197688231072
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0766000e+00 2.1525000e+00 -5.6454000e-01 /
CHEB / 4.7261000e+00 1.1488000e+00 5.7615000e-01 /
CHEB / -1.8111000e+00 6.8159000e-02 8.9607000e-02 /
CHEB / -9.1534000e-01 -1.0845000e-01 -3.2142000e-02 /
CHEB / -3.9514000e-01 -6.9119000e-02 -2.8679000e-02 /

C3H4O-enone+H(+m)=C2H4+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -14.648077497255036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0725000e+01 -1.0453000e+00 -1.5595000e-01 /
CHEB / 2.1805000e+00 1.0644000e+00 7.9120000e-02 /
CHEB / -5.6215000e-03 1.6644000e-01 1.0184000e-01 /
CHEB / -1.2951000e-01 -1.0777000e-01 2.2050000e-02 /
CHEB / -6.5813000e-02 -7.9329000e-02 -2.5915000e-02 /

C3H4O-enone+H(+m)=C2H5+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -35.28612585196037
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2279000e+00 -2.4884000e-02 -1.9733000e-02 /
CHEB / 1.7601000e+01 3.4151000e-02 2.6970000e-02 /
CHEB / 2.7406000e-01 -7.9146000e-03 -5.9768000e-03 /
CHEB / 7.8702000e-02 -2.6740000e-03 -2.3693000e-03 /
CHEB / 1.7940000e-02 8.2958000e-04 6.7239000e-04 /

C3H3OH+H(+m)=C3H5OJ(13)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -49.32455708010624
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5366000e+00 5.9259000e+00 -9.5663000e-01 /
CHEB / -1.5908000e+00 1.6245000e+00 8.2342000e-01 /
CHEB / -1.7840000e+00 -1.4640000e-01 4.5050000e-01 /
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CHEB / -8.6842000e-01 -3.4620000e-01 1.1663000e-01 /
CHEB / -4.0971000e-01 -1.8295000e-01 -2.0314000e-02 /

C3H3OH+H(+m)=C3H5OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -61.64310049609173
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2258000e+00 4.8827000e+00 -9.9769000e-01 /
CHEB / -3.2729000e+00 1.9408000e+00 8.1478000e-01 /
CHEB / -2.2535000e+00 1.2159000e-01 4.0978000e-01 /
CHEB / -1.0869000e+00 -1.7867000e-01 9.5609000e-02 /
CHEB / -5.4354000e-01 -9.9966000e-02 -3.0596000e-02 /

C3H3OH+H(+m)=C3H5O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond exact:
Ca_Cd/H/Nd     H_rad          deltaHrxn(T=298K) = -58.063496565785655
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7869000e+00 5.1634000e+00 -8.7793000e-01 /
CHEB / -3.5996000e+00 1.6997000e+00 6.9039000e-01 /
CHEB / -2.3781000e+00 1.0371000e-01 4.1363000e-01 /
CHEB / -1.1319000e+00 -1.8977000e-01 1.0360000e-01 /
CHEB / -5.5605000e-01 -1.1148000e-01 -3.3868000e-02 /

C3H3OH+H(+m)=CH2CHCH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -31.626153196259715
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2537000e+00 2.7997000e+00 -2.4464000e-01 /
CHEB / -1.2726000e+00 1.2823000e+00 5.1763000e-01 /
CHEB / -1.8026000e+00 8.1151000e-03 8.2719000e-02 /
CHEB / -9.2448000e-01 -1.3806000e-01 -2.2928000e-02 /
CHEB / -4.0675000e-01 -6.7887000e-02 -2.9261000e-02 /

C3H3OH+H(+m)=C2H4+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -33.05603300528368
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0841000e+01 -5.0766000e-01 -2.8494000e-01 /
CHEB / 1.6223000e+00 6.1833000e-01 3.2706000e-01 /
CHEB / -1.5671000e-01 -3.5103000e-02 9.4644000e-03 /
CHEB / -1.2692000e-01 -7.6547000e-02 -4.4962000e-02 /
CHEB / -6.8122000e-02 -1.6226000e-02 -1.6726000e-02 /

C3H3OH+H(+m)=C3H4O+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -18.78796671826114
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0803000e+01 -5.0712000e-01 -2.7467000e-01 /
CHEB / 1.4863000e+00 6.1217000e-01 3.1115000e-01 /
CHEB / -3.4944000e-02 -2.9560000e-02 1.3786000e-02 /
CHEB / -1.9811000e-02 -7.6034000e-02 -4.3515000e-02 /
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CHEB / 7.8263000e-04 -1.6297000e-02 -1.6545000e-02 /

C3H3OH+H(+m)=C2H5+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -53.69408135998901
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6130000e+00 -1.5303000e-01 -1.0131000e-01 /
CHEB / 1.1559000e+01 1.9201000e-01 1.2550000e-01 /
CHEB / 2.7704000e-01 -2.3631000e-02 -1.2927000e-02 /
CHEB / 6.0991000e-02 -1.7646000e-02 -1.2559000e-02 /
CHEB / -3.7147000e-03 -6.7386000e-04 -8.8166000e-04 /

C3H3OH+H(+m)=C3H4O-enone+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -18.407955508028643
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0787000e+01 -5.3828000e-01 -2.8686000e-01 /
CHEB / 1.3995000e+00 6.5041000e-01 3.2601000e-01 /
CHEB / -7.2144000e-02 -3.4546000e-02 1.1503000e-02 /
CHEB / -4.2936000e-02 -7.8104000e-02 -4.3882000e-02 /
CHEB / -1.1375000e-02 -1.6178000e-02 -1.6331000e-02 /

C3H3OH+H(+m)=C2H3+CH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -10.708348061150598
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6354000e+00 -4.4097000e-01 -2.1086000e-01 /
CHEB / 3.8468000e+00 5.6526000e-01 2.5344000e-01 /
CHEB / 5.1164000e-01 -8.5147000e-02 -1.4072000e-02 /
CHEB / 9.2502000e-02 -4.4869000e-02 -2.7691000e-02 /
CHEB / 1.5523000e-02 -3.6275000e-03 -6.4463000e-03 /

C2H3+CH2O(+m)=C3H5OJ(13)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -38.61620901895564
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.7123000e+00 5.7650000e+00 -1.0637000e+00 /
CHEB / 3.0763000e+00 1.8775000e+00 9.6930000e-01 /
CHEB / -1.4943000e+00 -1.8540000e-01 4.4075000e-01 /
CHEB / -8.0375000e-01 -3.7215000e-01 1.0296000e-01 /
CHEB / -3.8857000e-01 -1.8255000e-01 -2.0853000e-02 /

C2H3+CH2O(+m)=C3H5OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -50.93475243494113
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0243000e+00 4.7197000e+00 -1.1064000e+00 /
CHEB / 1.3951000e+00 2.1955000e+00 9.6186000e-01 /
CHEB / -1.9633000e+00 8.3751000e-02 4.0081000e-01 /
CHEB / -1.0226000e+00 -2.0497000e-01 8.1391000e-02 /
CHEB / -5.2271000e-01 -9.9717000e-02 -3.1542000e-02 /
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C2H3+CH2O(+m)=C3H5O-enol2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -47.35514850463505
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4690000e+00 4.9902000e+00 -9.9380000e-01 /
CHEB / 1.0744000e+00 1.9649000e+00 8.4417000e-01 /
CHEB / -2.0864000e+00 6.9070000e-02 4.0797000e-01 /
CHEB / -1.0695000e+00 -2.1957000e-01 8.6684000e-02 /
CHEB / -5.3576000e-01 -1.1235000e-01 -3.5982000e-02 /

C2H3+CH2O(+m)=CH2CHCH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd_pri_rad     CO/H2_O           deltaHrxn(T=298K)
= -20.917805135109113 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5350000e+00 1.1807000e+00 -1.7325000e-01 /
CHEB / -3.5558000e-02 7.8512000e-01 1.3214000e-01 /
CHEB / -1.7094000e+00 1.6459000e-01 5.8293000e-02 /
CHEB / -8.8881000e-01 -4.1078000e-02 -1.5159000e-03 /
CHEB / -4.0290000e-01 -5.6048000e-02 -1.4848000e-02 /

C2H3+CH2O(+m)=C2H4+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -22.34768494413308
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7045000e+00 -6.7284000e-01 -3.7722000e-01 /
CHEB / 6.3705000e+00 8.4515000e-01 4.5222000e-01 /
CHEB / 1.8181000e-01 -8.5674000e-02 -1.5700000e-02 /
CHEB / -2.4443000e-02 -9.6694000e-02 -5.7752000e-02 /
CHEB / -2.8568000e-02 -1.0673000e-02 -1.4021000e-02 /

C2H3+CH2O(+m)=C3H4O+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -8.079618657110544
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6241000e+00 -6.4454000e-01 -1.5240000e-01 /
CHEB / 3.3450000e+00 7.4817000e-01 1.5229000e-01 /
CHEB / 1.5813000e-01 3.6928000e-03 3.3249000e-02 /
CHEB / 1.3400000e-01 -9.5973000e-02 -2.1355000e-02 /
CHEB / 1.1219000e-01 -3.1189000e-02 -1.4733000e-02 /

C2H3+CH2O(+m)=C2H5+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -42.98573329883841
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4854000e+00 -1.5832000e-01 -1.0415000e-01 /
CHEB / 1.6138000e+01 1.9835000e-01 1.2875000e-01 /
CHEB / 6.4438000e-01 -2.4014000e-02 -1.2923000e-02 /
CHEB / 1.6616000e-01 -1.8323000e-02 -1.2936000e-02 /
CHEB / 2.8851000e-02 -7.9697000e-04 -9.9714000e-04 /
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C2H3+CH2O(+m)=C3H4O-enone+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -7.699607446878041
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6620000e+00 -6.9583000e-01 -3.7575000e-01 /
CHEB / 6.1488000e+00 8.7032000e-01 4.4840000e-01 /
CHEB / 2.6833000e-01 -8.8074000e-02 -1.5370000e-02 /
CHEB / 6.2075000e-02 -9.6376000e-02 -5.5826000e-02 /
CHEB / 2.8602000e-02 -9.7901000e-03 -1.3143000e-02 /

aC3H5+O(+m)=C3H5OJ(13)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -94.31050402801606
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2132000e+01 1.5259000e+01 2.1404000e-01 /
CHEB / -3.6322000e+00 -2.0690000e+00 1.4730000e+00 /
CHEB / -1.6529000e+00 -1.5310000e+00 -1.4189000e-01 /
CHEB / -7.0858000e-01 -6.9913000e-01 -1.5476000e-01 /
CHEB / -3.8431000e-01 -2.1789000e-01 6.3736000e-02 /

aC3H5+O(+m)=C3H5OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -106.62904744400156
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8376000e+00 1.4937000e+01 -4.5640000e-01 /
CHEB / -5.2868000e+00 -1.7837000e+00 1.5164000e+00 /
CHEB / -1.7506000e+00 -1.9719000e+00 4.2293000e-01 /
CHEB / -8.0919000e-01 -7.6211000e-01 1.7617000e-02 /
CHEB / -6.1397000e-01 4.3378000e-02 -9.5897000e-02 /

aC3H5+O(+m)=C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -103.04944351369548
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3197000e+00 1.5105000e+01 -3.8911000e-01 /
CHEB / -5.5397000e+00 -1.9068000e+00 1.4845000e+00 /
CHEB / -1.9057000e+00 -1.9787000e+00 3.8922000e-01 /
CHEB / -8.7093000e-01 -7.6724000e-01 -2.8225000e-03 /
CHEB / -6.1282000e-01 8.6091000e-03 -7.8206000e-02 /

aC3H5+O(+m)=CH2CHCH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: Oa_R_Recombination estimate:
(Average:) C_rad/H2/Cd     Oa       deltaHrxn(T=298K) = -
76.61210014416955 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9263000e+00 8.3637000e+00 1.7723000e+00 /
CHEB / -2.6003000e+00 -1.2780000e+00 -7.7582000e-01 /
CHEB / -1.0229000e+00 -7.0292000e-01 -6.2600000e-01 /
CHEB / -5.1444000e-01 -4.1675000e-01 -1.0665000e-01 /
CHEB / -3.7773000e-01 -2.4008000e-01 1.6449000e-01 /
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aC3H5+O(+m)=C2H4+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -78.04197995319349
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7890000e+00 4.9368000e-03 1.1843000e-03 /
CHEB / 8.3581000e-01 -1.2839000e-03 2.7125000e-03 /
CHEB / 3.8367000e-02 -6.7891000e-03 -6.4213000e-03 /
CHEB / -5.4832000e-02 2.6801000e-03 2.0956000e-03 /
CHEB / -5.1861000e-02 1.0607000e-03 9.2491000e-04 /

aC3H5+O(+m)=C3H4O+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -63.77391366617096 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4682000e+00 -7.0848000e-04 -8.9101000e-04 /
CHEB / 3.4056000e-01 2.0059000e-03 1.9864000e-03 /
CHEB / 1.1828000e-01 -1.5018000e-03 -1.2405000e-03 /
CHEB / 5.0224000e-02 -9.1396000e-05 -9.9939000e-05 /
CHEB / 1.8933000e-02 3.2900000e-04 2.7363000e-04 /

aC3H5+O(+m)=C2H5+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -98.68002830789884 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4954000e+00 -9.7083000e-02 -6.4983000e-02 /
CHEB / 3.1302000e+00 1.2577000e-01 8.3541000e-02 /
CHEB / 8.6148000e-01 -2.1024000e-02 -1.2962000e-02 /
CHEB / 2.2506000e-01 -1.0214000e-02 -7.2581000e-03 /
CHEB / 4.2905000e-02 9.1787000e-04 4.8498000e-04 /

aC3H5+O(+m)=C3H4O-enone+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -63.393902455938466
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0508000e+00 -5.0055000e-03 -5.8158000e-03 /
CHEB / 4.9570000e-01 1.0838000e-02 1.1162000e-02 /
CHEB / 9.5572000e-02 -7.9110000e-03 -7.0298000e-03 /
CHEB / 2.9852000e-02 1.3916000e-03 1.0775000e-03 /
CHEB / 8.6552000e-03 1.0476000e-03 9.0848000e-04 /

aC3H5+O(+m)=C3H3OH+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -44.98594694790983
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7099000e+00 -4.1322000e-02 -2.9125000e-02 /
CHEB / 9.4866000e-01 5.3676000e-02 3.7793000e-02 /
CHEB / 3.0929000e-01 -9.1592000e-03 -6.3412000e-03 /
CHEB / 1.1032000e-01 -4.1732000e-03 -3.0546000e-03 /
CHEB / 3.1502000e-02 3.6372000e-04 2.8249000e-04 /

aC3H5+O(+m)=C2H3+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -55.694295009060426
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.3098000e+01 -1.3520000e-06 -9.4144000e-07 /
CHEB / -6.8036000e-02 1.4752000e-06 1.0272000e-06 /
CHEB / 3.1680000e-03 2.4330000e-07 1.6944000e-07 /
CHEB / 1.2190000e-02 -2.2842000e-07 -1.5905000e-07 /
CHEB / 7.0690000e-03 -2.4579000e-07 -1.7115000e-07 /

pC3H5+O(+m)=C3H5OJ(13)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -117.77804597967713
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6634000e+01 1.7438000e+01 2.5198000e+00 /
CHEB / -4.5360000e+00 -3.4716000e+00 3.8166000e-01 /
CHEB / -1.8477000e+00 -1.3647000e+00 -6.6749000e-01 /
CHEB / -7.0679000e-01 -4.7588000e-01 -3.7227000e-01 /
CHEB / -3.2624000e-01 -1.8045000e-01 -3.7022000e-02 /

pC3H5+O(+m)=C3H5OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Cd_pri_rad     Oa        deltaHrxn(T=298K) = -
130.09658939566265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4438000e+01 1.8895000e+01 1.0287000e+00 /
CHEB / -5.8328000e+00 -3.8458000e+00 9.3791000e-01 /
CHEB / -1.6107000e+00 -2.1323000e+00 -5.1527000e-01 /
CHEB / -5.9219000e-01 -8.4801000e-01 -1.6075000e-01 /
CHEB / -4.4238000e-01 -2.0620000e-01 2.0523000e-01 /

pC3H5+O(+m)=C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -126.51698546535656
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4904000e+01 1.9034000e+01 1.1182000e+00 /
CHEB / -6.0883000e+00 -3.9629000e+00 9.0002000e-01 /
CHEB / -1.7683000e+00 -2.1370000e+00 -5.4569000e-01 /
CHEB / -6.5981000e-01 -8.4332000e-01 -1.8634000e-01 /
CHEB / -4.5639000e-01 -2.1039000e-01 1.9297000e-01 /

pC3H5+O(+m)=CH2CHCH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -100.07964209583062
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6452000e+01 1.3417000e+01 3.1252000e+00 /
CHEB / -4.7508000e+00 -3.5113000e+00 -4.4369000e-01 /
CHEB / -1.6506000e+00 -1.2994000e+00 -9.4293000e-01 /
CHEB / -5.6914000e-01 -4.6355000e-01 -3.8664000e-01 /
CHEB / -2.5033000e-01 -1.9336000e-01 3.0598000e-02 /

pC3H5+O(+m)=C2H4+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -101.50952190485457
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.2431000e+01 5.7891000e-04 4.1368000e-04 /
CHEB / 9.5369000e-02 -7.0495000e-04 -5.0625000e-04 /
CHEB / -7.8410000e-02 9.8510000e-05 7.3547000e-05 /
CHEB / -5.7732000e-02 4.3135000e-05 3.0502000e-05 /
CHEB / -3.8608000e-02 -9.3983000e-07 -1.3293000e-06 /

pC3H5+O(+m)=C3H4O+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -87.24145561783206 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2560000e+01 4.6809000e-04 3.3199000e-04 /
CHEB / -7.0952000e-02 -5.9160000e-04 -4.2039000e-04 /
CHEB / 3.8472000e-02 8.0706000e-05 5.8233000e-05 /
CHEB / 5.4676000e-02 4.6260000e-05 3.3129000e-05 /
CHEB / 3.3425000e-02 8.0358000e-07 -2.1284000e-08 /

pC3H5+O(+m)=C2H5+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -122.14757025955991 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3867000e+00 -5.5591000e-03 -3.8714000e-03 /
CHEB / 1.7062000e+00 6.6097000e-03 4.6033000e-03 /
CHEB / 5.5787000e-01 -7.1320000e-04 -4.9680000e-04 /
CHEB / 2.0208000e-01 -3.5263000e-04 -2.4586000e-04 /
CHEB / 6.1337000e-02 -4.0033000e-05 -2.7735000e-05 /

pC3H5+O(+m)=C3H4O-enone+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -86.86144440759955
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2770000e+01 1.6458000e-04 1.1956000e-04 /
CHEB / -2.5664000e-01 -2.1467000e-04 -1.5647000e-04 /
CHEB / -1.8971000e-02 3.1191000e-05 2.3526000e-05 /
CHEB / 3.0762000e-02 2.1468000e-05 1.5590000e-05 /
CHEB / 2.3955000e-02 -1.1881000e-06 -1.2680000e-06 /

pC3H5+O(+m)=C3H3OH+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -68.45348889957091
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1444000e+01 -4.8591000e-03 -3.5340000e-03 /
CHEB / -2.1958000e-01 6.1590000e-03 4.5152000e-03 /
CHEB / -6.0521000e-02 -1.0057000e-03 -7.8850000e-04 /
CHEB / 1.8423000e-03 -2.7189000e-04 -1.8095000e-04 /
CHEB / 5.2237000e-03 -5.4019000e-05 -3.3301000e-05 /

pC3H5+O(+m)=C2H3+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -79.1618369607215
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0316000e+01 -6.7851000e-03 -4.8782000e-03 /
CHEB / 8.0642000e-02 8.4997000e-03 6.1489000e-03 /
CHEB / 2.6881000e-02 -1.2741000e-03 -9.7528000e-04 /
CHEB / 2.9313000e-02 -4.2338000e-04 -2.8786000e-04 /
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CHEB / 1.9416000e-02 -7.0706000e-05 -4.4401000e-05 /

pC3H5+O(+m)=aC3H5+O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -23.467541951661083 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7296000e+00 -3.2778000e-02 -2.2627000e-02 /
CHEB / 1.2176000e+00 4.1933000e-02 2.8902000e-02 /
CHEB / 5.7614000e-01 -6.6091000e-03 -4.4883000e-03 /
CHEB / 2.4134000e-01 -3.0573000e-03 -2.1375000e-03 /
CHEB / 8.8965000e-02 1.6153000e-06 -5.3437000e-06 /

C3H5OJ(13)(+m)=C3H5OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    C_rad_out_2H     CO_H_out
      deltaHrxn(T=298K) = -13.538390170974031 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5566000e+00 1.2194000e+00 -2.4971000e-01 /
CHEB / 9.1684000e+00 1.1638000e+00 8.6609000e-02 /
CHEB / -1.1049000e+00 3.1719000e-01 -1.6996000e-02 /
CHEB / -7.5268000e-01 -5.8578000e-03 1.1906000e-02 /
CHEB / -3.9364000e-01 -7.6748000e-02 2.0976000e-02 /

C3H5OJ(13)(+m)=C3H5OJ(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 19.7281679202151
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0964000e+01 7.1221000e+00 -9.7714000e-01 /
CHEB / 1.6519000e+01 1.2774000e+00 1.0354000e+00 /
CHEB / -1.7606000e+00 -3.8619000e-01 4.9768000e-01 /
CHEB / -8.6163000e-01 -4.2947000e-01 1.1899000e-01 /
CHEB / -4.2719000e-01 -1.8085000e-01 -2.8039000e-02 /

C3H5OJ(13)(+m)=CHCHCH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 21.92794329312682
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0830000e+01 6.9878000e+00 -9.7698000e-01 /
CHEB / 1.6432000e+01 1.3192000e+00 1.0138000e+00 /
CHEB / -1.7413000e+00 -3.5908000e-01 4.9349000e-01 /
CHEB / -8.5756000e-01 -4.2033000e-01 1.1907000e-01 /
CHEB / -4.2450000e-01 -1.8126000e-01 -2.7148000e-02 /

C3H5OJ(13)(+m)=C3H5OJ(17)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 14.88860613724357
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5930000e+00 1.1532000e+00 -2.9957000e-01 /
CHEB / 9.1695000e+00 1.1673000e+00 9.2432000e-02 /
CHEB / -1.0693000e+00 3.8257000e-01 3.3117000e-02 /
CHEB / -7.5135000e-01 -3.9813000e-03 1.1957000e-02 /
CHEB / -4.0555000e-01 -9.8242000e-02 5.1607000e-03 /
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C3H5OJ(13)(+m)=CH3CHcOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 14.258649429223652
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5930000e+00 1.1532000e+00 -2.9956000e-01 /
CHEB / 9.1695000e+00 1.1673000e+00 9.2450000e-02 /
CHEB / -1.0693000e+00 3.8258000e-01 3.3130000e-02 /
CHEB / -7.5135000e-01 -3.9722000e-03 1.1964000e-02 /
CHEB / -4.0555000e-01 -9.8239000e-02 5.1631000e-03 /

C3H5OJ(12)(+m)=C3H5OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_H/NonDeC     CO_H_out
      deltaHrxn(T=298K) = -1.2198467549885343 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8045000e+00 5.2079000e-01 -3.5118000e-02 /
CHEB / 1.0447000e+01 7.6894000e-01 -3.2418000e-02 /
CHEB / -1.2495000e+00 4.5678000e-01 3.2369000e-03 /
CHEB / -8.5926000e-01 1.6319000e-01 3.3533000e-02 /
CHEB / -5.0124000e-01 -1.3998000e-02 2.8328000e-02 /

C3H5OJ(12)(+m)=C3H5OJ(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 32.046711336200595
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1436000e+01 6.0763000e+00 -1.0260000e+00 /
CHEB / 1.9061000e+01 1.6068000e+00 1.0256000e+00 /
CHEB / -2.2416000e+00 -1.1295000e-01 4.5486000e-01 /
CHEB / -1.0993000e+00 -2.6194000e-01 9.7298000e-02 /
CHEB / -5.7001000e-01 -1.0079000e-01 -3.5727000e-02 /

C3H5OJ(12)(+m)=CHCHCH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 34.24648670911232
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1302000e+01 5.9418000e+00 -1.0250000e+00 /
CHEB / 1.8975000e+01 1.6470000e+00 1.0044000e+00 /
CHEB / -2.2221000e+00 -8.6252000e-02 4.5084000e-01 /
CHEB / -1.0954000e+00 -2.5237000e-01 9.7110000e-02 /
CHEB / -5.6775000e-01 -1.0028000e-01 -3.5558000e-02 /

C3H5OJ(12)(+m)=C3H5OJ(17)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) R3H_SD     O_rad_out     Cd_H_out_singleNd
      deltaHrxn(T=298K) = 27.207149553229065 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8053000e+00 5.1960000e-01 -3.5795000e-02 /
CHEB / 1.0446000e+01 7.6668000e-01 -3.3706000e-02 /
CHEB / -1.2506000e+00 4.5486000e-01 2.1329000e-03 /
CHEB / -8.6013000e-01 1.6173000e-01 3.2684000e-02 /
CHEB / -5.0182000e-01 -1.4982000e-02 2.7747000e-02 /
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C3H5OJ(12)(+m)=CH3CHcOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    O_rad_out     Cd_H_out_doubleC
      deltaHrxn(T=298K) = 26.577192845209147 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8053000e+00 5.1961000e-01 -3.5788000e-02 /
CHEB / 1.0446000e+01 7.6670000e-01 -3.3693000e-02 /
CHEB / -1.2506000e+00 4.5487000e-01 2.1429000e-03 /
CHEB / -8.6013000e-01 1.6174000e-01 3.2689000e-02 /
CHEB / -5.0182000e-01 -1.4980000e-02 2.7749000e-02 /

C3H5O-enol2(+m)=C3H5OJ(8)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -4.7994506852946115
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1998000e+00 -1.5557000e-01 -2.5241000e-01 /
CHEB / 9.4835000e+00 1.5726000e+00 1.5161000e-01 /
CHEB / -1.4361000e+00 4.9815000e-01 9.6206000e-02 /
CHEB / -9.9336000e-01 4.1004000e-02 1.5113000e-02 /
CHEB / -5.4039000e-01 -8.1254000e-02 -1.0037000e-02 /

C3H5O-enol2(+m)=C3H5OJ(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 28.467107405894517
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0193000e+01 6.3204000e+00 -9.2922000e-01 /
CHEB / 1.7377000e+01 1.4109000e+00 9.2721000e-01 /
CHEB / -2.4375000e+00 -1.3391000e-01 4.6102000e-01 /
CHEB / -1.1579000e+00 -2.7932000e-01 9.9811000e-02 /
CHEB / -5.7903000e-01 -1.1330000e-01 -4.0545000e-02 /

C3H5O-enol2(+m)=CHCHCH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 30.666882778806237
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0056000e+01 6.1894000e+00 -9.2589000e-01 /
CHEB / 1.7288000e+01 1.4469000e+00 9.0330000e-01 /
CHEB / -2.4177000e+00 -1.0678000e-01 4.5695000e-01 /
CHEB / -1.1536000e+00 -2.6916000e-01 1.0018000e-01 /
CHEB / -5.7675000e-01 -1.1275000e-01 -4.0299000e-02 /

C3H5O-enol2(+m)=C3H5OJ(17)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 23.627545622922987
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2006000e+00 -1.5681000e-01 -2.5312000e-01 /
CHEB / 9.4821000e+00 1.5703000e+00 1.5027000e-01 /
CHEB / -1.4373000e+00 4.9618000e-01 9.5071000e-02 /
CHEB / -9.9424000e-01 3.9532000e-02 1.4253000e-02 /
CHEB / -5.4097000e-01 -8.2237000e-02 -1.0618000e-02 /
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C3H5O-enol2(+m)=CH3CHcOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 22.99758891490307
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2006000e+00 -1.5680000e-01 -2.5311000e-01 /
CHEB / 9.4821000e+00 1.5703000e+00 1.5028000e-01 /
CHEB / -1.4373000e+00 4.9620000e-01 9.5081000e-02 /
CHEB / -9.9423000e-01 3.9538000e-02 1.4258000e-02 /
CHEB / -5.4097000e-01 -8.2236000e-02 -1.0617000e-02 /

CH2CHCH2O(+m)=C3H5OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -31.236794054820553
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8526000e+00 2.1895000e+00 -5.7536000e-01 /
CHEB / 9.3626000e+00 1.0379000e+00 5.6135000e-01 /
CHEB / -1.7669000e+00 5.0268000e-02 8.2577000e-02 /
CHEB / -9.1214000e-01 -1.0709000e-01 -3.3926000e-02 /
CHEB / -3.9587000e-01 -6.8802000e-02 -2.9655000e-02 /

CH2CHCH2O(+m)=C3H5OJ(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     Cd_H_out_doubleC
      deltaHrxn(T=298K) = 2.029764036368576 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6978000e+00 2.7038000e+00 -2.7651000e-01 /
CHEB / 8.8065000e+00 4.8675000e-01 2.5575000e-01 /
CHEB / -1.8296000e+00 5.0061000e-02 5.8258000e-02 /
CHEB / -9.2836000e-01 -5.8664000e-02 -7.5397000e-03 /
CHEB / -4.1458000e-01 -5.0798000e-02 -1.5582000e-02 /

CH2CHCH2O(+m)=CHCHCH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13)) High-P Limit: intra_H_migration estimate:
(Average:) R4H_SSD     O_rad_out     Cd_H_out_singleH
      deltaHrxn(T=298K) = 4.229539409280296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0958000e+00 2.7038000e+00 -2.7651000e-01 /
CHEB / 8.8065000e+00 4.8674000e-01 2.5574000e-01 /
CHEB / -1.8296000e+00 5.0057000e-02 5.8255000e-02 /
CHEB / -9.2836000e-01 -5.8665000e-02 -7.5406000e-03 /
CHEB / -4.1458000e-01 -5.0798000e-02 -1.5582000e-02 /

CH2CHCH2O(+m)=C3H5OJ(17)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -2.8097977466029533
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8593000e+00 2.1877000e+00 -5.7613000e-01 /
CHEB / 9.3504000e+00 1.0344000e+00 5.5986000e-01 /
CHEB / -1.7763000e+00 4.7346000e-02 8.1295000e-02 /
CHEB / -9.1847000e-01 -1.0925000e-01 -3.4905000e-02 /
CHEB / -3.9964000e-01 -7.0209000e-02 -3.0321000e-02 /
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CH2CHCH2O(+m)=CH3CHcOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -3.4397544546228715
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8589000e+00 2.1883000e+00 -5.7576000e-01 /
CHEB / 9.3508000e+00 1.0351000e+00 5.6025000e-01 /
CHEB / -1.7762000e+00 4.7510000e-02 8.1395000e-02 /
CHEB / -9.1847000e-01 -1.0927000e-01 -3.4916000e-02 /
CHEB / -3.9967000e-01 -7.0260000e-02 -3.0351000e-02 /

C2H4+HCO(+m)=C3H5OJ(8)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -29.80691424579659
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4748000e+00 -1.1880000e+00 -7.1541000e-02 /
CHEB / 6.4107000e+00 1.1574000e+00 3.0846000e-02 /
CHEB / 2.2403000e-01 1.9570000e-01 4.7477000e-03 /
CHEB / -4.7032000e-02 -4.5977000e-02 6.3696000e-02 /
CHEB / -1.3702000e-02 -8.2137000e-02 9.7915000e-03 /

C2H4+HCO(+m)=C3H5OJ(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = 3.459643845392538 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.4070000e+00 -3.5743000e-01 -2.2474000e-01 /
CHEB / 1.5033000e+01 4.5094000e-01 2.7150000e-01 /
CHEB / 8.9701000e-02 -4.5093000e-02 -9.7421000e-03 /
CHEB / -5.2559000e-02 -5.5006000e-02 -3.6984000e-02 /
CHEB / -5.1470000e-02 -6.3895000e-03 -9.3359000e-03 /

C2H4+HCO(+m)=CHCHCH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 5.659419218304258
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.4205000e+00 -3.7221000e-01 -2.3142000e-01 /
CHEB / 1.4928000e+01 4.6773000e-01 2.7811000e-01 /
CHEB / 1.1062000e-01 -4.4448000e-02 -8.1510000e-03 /
CHEB / -4.6055000e-02 -5.7238000e-02 -3.7914000e-02 /
CHEB / -4.8712000e-02 -7.2849000e-03 -1.0065000e-02 /

C2H4+HCO(+m)=C3H5OJ(17)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -1.3799179375789912
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3344000e+00 -1.3373000e+00 -1.6860000e-01 /
CHEB / 6.3628000e+00 1.2477000e+00 9.7507000e-02 /
CHEB / 2.1570000e-01 3.0252000e-01 6.5401000e-02 /
CHEB / -1.0376000e-01 -7.0468000e-02 4.4643000e-02 /
CHEB / -4.7476000e-02 -1.0546000e-01 -2.2358000e-03 /

C2H4+HCO(+m)=CH3CHcOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -2.0098746455989094
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3399000e+00 -1.3372000e+00 -1.6855000e-01 /
CHEB / 6.3734000e+00 1.2478000e+00 9.7576000e-02 /
CHEB / 2.2514000e-01 3.0256000e-01 6.5429000e-02 /
CHEB / -9.5965000e-02 -7.0504000e-02 4.4622000e-02 /
CHEB / -4.1549000e-02 -1.0555000e-01 -2.2903000e-03 /

C3H4O+H(+m)=C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -44.074980532819126
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1224000e+01 -1.1073000e+00 -8.7308000e-02 /
CHEB / 1.2351000e+00 1.0297000e+00 -8.0313000e-03 /
CHEB / 3.6899000e-02 2.7300000e-01 9.1556000e-02 /
CHEB / -3.4830000e-02 -7.0507000e-02 5.1319000e-02 /
CHEB / 2.1556000e-02 -1.0055000e-01 -1.1460000e-02 /

C3H4O+H(+m)=C3H5OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -10.808422441629993 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9955000e+00 -3.5416000e-01 -2.1501000e-01 /
CHEB / 9.4754000e+00 4.3730000e-01 2.5323000e-01 /
CHEB / -3.9831000e-02 -3.0998000e-02 2.0565000e-04 /
CHEB / -3.5214000e-02 -5.8900000e-02 -3.8560000e-02 /
CHEB / -8.6606000e-03 -5.4073000e-03 -8.4428000e-03 /

C3H4O+H(+m)=CHCHCH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -8.608647068718273
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9952000e+00 -3.5415000e-01 -2.1199000e-01 /
CHEB / 9.3436000e+00 4.2937000e-01 2.4387000e-01 /
CHEB / -3.0969000e-03 -1.6076000e-02 1.0617000e-02 /
CHEB / -3.4730000e-02 -6.6670000e-02 -4.2670000e-02 /
CHEB / -4.2442000e-03 -5.0843000e-03 -8.6339000e-03 /

C3H4O+H(+m)=C3H5OJ(17)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -15.647984224601522
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1209000e+01 -1.1076000e+00 -8.7458000e-02 /
CHEB / 1.2066000e+00 1.0294000e+00 -8.2161000e-03 /
CHEB / 1.3359000e-02 2.7311000e-01 9.1593000e-02 /
CHEB / -5.1814000e-02 -7.0165000e-02 5.1497000e-02 /
CHEB / 1.1049000e-02 -1.0025000e-01 -1.1278000e-02 /

C3H4O+H(+m)=CH3CHcOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -16.27794093262144
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1216000e+01 -1.1075000e+00 -8.7421000e-02 /
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CHEB / 1.2203000e+00 1.0294000e+00 -8.1587000e-03 /
CHEB / 2.5322000e-02 2.7312000e-01 9.1610000e-02 /
CHEB / -4.2236000e-02 -7.0211000e-02 5.1469000e-02 /
CHEB / 1.8023000e-02 -1.0033000e-01 -1.1335000e-02 /

C2H5+CO(+m)=C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -9.168865891091254
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4656000e+01 -1.1218000e-03 -1.6561000e-03 /
CHEB / 3.0273000e+01 2.3306000e-03 2.8168000e-03 /
CHEB / 5.5867000e-01 -1.4015000e-03 -1.1817000e-03 /
CHEB / 1.7496000e-01 -2.9744000e-04 -4.1926000e-04 /
CHEB / 5.0191000e-02 4.5433000e-04 3.8269000e-04 /

C2H5+CO(+m)=C3H5OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = 24.097692200097875 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6145000e+01 -1.6946000e-01 -1.0995000e-01 /
CHEB / 3.0577000e+01 2.1246000e-01 1.3577000e-01 /
CHEB / 6.1277000e-01 -2.5695000e-02 -1.3274000e-02 /
CHEB / 1.5738000e-01 -1.9892000e-02 -1.3876000e-02 /
CHEB / 1.9379000e-02 -8.0832000e-04 -1.1132000e-03 /

C2H5+CO(+m)=CHCHCH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 26.297467573009595
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6311000e+01 -1.6761000e-01 -1.0900000e-01 /
CHEB / 3.0625000e+01 2.1011000e-01 1.3461000e-01 /
CHEB / 6.2266000e-01 -2.5398000e-02 -1.3203000e-02 /
CHEB / 1.6172000e-01 -1.9640000e-02 -1.3728000e-02 /
CHEB / 2.1587000e-02 -8.0921000e-04 -1.0964000e-03 /

C2H5+CO(+m)=C3H5OJ(17)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 19.258130417126345
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5207000e+01 -1.1728000e-02 -1.1684000e-02 /
CHEB / 3.0472000e+01 1.7110000e-02 1.7027000e-02 /
CHEB / 5.8504000e-01 -6.1282000e-03 -5.7296000e-03 /
CHEB / 1.9089000e-01 -4.0082000e-04 -7.8221000e-04 /
CHEB / 5.6569000e-02 1.3497000e-03 1.2640000e-03 /

C2H5+CO(+m)=CH3CHcOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = 18.628173709106427
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5133000e+01 -2.7194000e-02 -2.0400000e-02 /
CHEB / 3.0485000e+01 3.4186000e-02 2.5940000e-02 /
CHEB / 5.7506000e-01 -5.2686000e-03 -4.2393000e-03 /
CHEB / 1.7421000e-01 -2.2696000e-03 -1.8936000e-03 /
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CHEB / 4.2754000e-02 4.7048000e-04 5.1414000e-04 /

C3H4O-enone+H(+m)=C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -44.45499174305163
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0142000e+01 -1.0177000e+00 -1.1540000e-01 /
CHEB / 1.7754000e+00 9.9381000e-01 2.2061000e-02 /
CHEB / 2.8784000e-02 2.0564000e-01 1.0654000e-01 /
CHEB / -2.2334000e-02 -8.4529000e-02 3.7740000e-02 /
CHEB / 1.7254000e-02 -8.6547000e-02 -2.1791000e-02 /

C3H4O-enone+H(+m)=C3H5OJ(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -11.188433651862496
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5354000e+00 -3.8886000e-01 -2.3253000e-01 /
CHEB / 9.3805000e+00 4.8275000e-01 2.7647000e-01 /
CHEB / -2.1991000e-02 -4.2212000e-02 -6.5100000e-03 /
CHEB / -2.9792000e-02 -5.6840000e-02 -3.6502000e-02 /
CHEB / -1.4852000e-02 -7.3766000e-03 -9.5278000e-03 /

C3H4O-enone+H(+m)=CHCHCH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -8.988658278950776
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5155000e+00 -4.0370000e-01 -2.3871000e-01 /
CHEB / 9.2788000e+00 4.9964000e-01 2.8251000e-01 /
CHEB / -2.9000000e-04 -4.1706000e-02 -4.9748000e-03 /
CHEB / -2.3190000e-02 -5.9032000e-02 -3.7377000e-02 /
CHEB / -1.2101000e-02 -8.1937000e-03 -1.0201000e-02 /

C3H4O-enone+H(+m)=C3H5OJ(17)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -16.027995434834025
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0132000e+01 -1.0178000e+00 -1.1542000e-01 /
CHEB / 1.7573000e+00 9.9378000e-01 2.2034000e-02 /
CHEB / 1.4196000e-02 2.0571000e-01 1.0657000e-01 /
CHEB / -3.2366000e-02 -8.4408000e-02 3.7795000e-02 /
CHEB / 1.1616000e-02 -8.6472000e-02 -2.1740000e-02 /

C3H4O-enone+H(+m)=CH3CHcOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -16.657952142853944
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0140000e+01 -1.0178000e+00 -1.1540000e-01 /
CHEB / 1.7710000e+00 9.9383000e-01 2.2074000e-02 /
CHEB / 2.6018000e-02 2.0570000e-01 1.0657000e-01 /
CHEB / -2.3157000e-02 -8.4454000e-02 3.7767000e-02 /
CHEB / 1.8042000e-02 -8.6531000e-02 -2.1784000e-02 /
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C3H3OH+H(+m)=C3H5OJ(8)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -62.86294725108027
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8203000e+00 -4.6369000e-01 -2.7801000e-01 /
CHEB / 1.5833000e+00 5.7526000e-01 3.2489000e-01 /
CHEB / -3.3907000e-02 -4.1260000e-02 4.2920000e-03 /
CHEB / 6.3850000e-04 -7.4586000e-02 -4.6340000e-02 /
CHEB / 2.3059000e-02 -1.4689000e-02 -1.6437000e-02 /

C3H3OH+H(+m)=C3H5OJ(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -29.59638915989114 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7643000e+00 -2.9957000e-01 -1.4569000e-01 /
CHEB / 4.3804000e+00 3.6392000e-01 1.6398000e-01 /
CHEB / 3.7733000e-01 -2.3929000e-02 7.7395000e-03 /
CHEB / 6.2339000e-02 -4.2228000e-02 -2.2892000e-02 /
CHEB / -4.0101000e-03 -6.5292000e-03 -8.1915000e-03 /

C3H3OH+H(+m)=CHCHCH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -27.39661378697942
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6929000e+00 -3.0690000e-01 -1.4707000e-01 /
CHEB / 4.3203000e+00 3.7330000e-01 1.6508000e-01 /
CHEB / 4.0313000e-01 -2.5410000e-02 8.4777000e-03 /
CHEB / 6.8033000e-02 -4.2798000e-02 -2.3173000e-02 /
CHEB / -1.4434000e-03 -6.6473000e-03 -8.4355000e-03 /

C3H3OH+H(+m)=C3H5OJ(17)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -34.43595094286267
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9435000e+00 -4.6383000e-01 -2.7810000e-01 /
CHEB / 1.8164000e+00 5.7489000e-01 3.2466000e-01 /
CHEB / 1.6242000e-01 -4.1619000e-02 4.0448000e-03 /
CHEB / 1.4664000e-01 -7.4665000e-02 -4.6433000e-02 /
CHEB / 1.1748000e-01 -1.4400000e-02 -1.6274000e-02 /

C3H3OH+H(+m)=CH3CHcOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -35.065907650882586
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9790000e+00 -4.6392000e-01 -2.7803000e-01 /
CHEB / 1.8762000e+00 5.7449000e-01 3.2448000e-01 /
CHEB / 1.9574000e-01 -4.1818000e-02 3.7733000e-03 /
CHEB / 1.5147000e-01 -7.4404000e-02 -4.6433000e-02 /
CHEB / 1.0212000e-01 -1.3944000e-02 -1.6028000e-02 /

C2H3+CH2O(+m)=C3H5OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -52.15459918992967
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6765000e+00 -6.3672000e-01 -3.7405000e-01 /
CHEB / 6.3379000e+00 8.0865000e-01 4.5291000e-01 /
CHEB / 3.0925000e-01 -8.8170000e-02 -1.8751000e-02 /
CHEB / 1.0481000e-01 -9.6453000e-02 -5.9964000e-02 /
CHEB / 6.4431000e-02 -1.0158000e-02 -1.4323000e-02 /

C2H3+CH2O(+m)=C3H5OJ(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -18.888041098740537
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9461000e+00 -2.0511000e-01 -1.1521000e-01 /
CHEB / 6.0109000e+00 2.6493000e-01 1.4445000e-01 /
CHEB / 3.8697000e-01 -3.5488000e-02 -1.2922000e-02 /
CHEB / 1.4812000e-01 -3.1631000e-02 -1.9196000e-02 /
CHEB / 6.9250000e-02 5.7498000e-04 -1.4545000e-03 /

C2H3+CH2O(+m)=CHCHCH2OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -16.688265725828817
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5407000e+00 -2.0509000e-01 -1.1520000e-01 /
CHEB / 5.9968000e+00 2.6495000e-01 1.4446000e-01 /
CHEB / 3.7523000e-01 -3.5487000e-02 -1.2920000e-02 /
CHEB / 1.3947000e-01 -3.1644000e-02 -1.9205000e-02 /
CHEB / 6.3654000e-02 5.5933000e-04 -1.4652000e-03 /

C2H3+CH2O(+m)=C3H5OJ(17)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -23.727602881712066
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8147000e+00 -6.3683000e-01 -3.7411000e-01 /
CHEB / 6.5985000e+00 8.0826000e-01 4.5268000e-01 /
CHEB / 5.2633000e-01 -8.8594000e-02 -1.9053000e-02 /
CHEB / 2.6303000e-01 -9.6563000e-02 -6.0090000e-02 /
CHEB / 1.6325000e-01 -9.8401000e-03 -1.4144000e-02 /

C2H3+CH2O(+m)=CH3CHcOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -24.357559589731984
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8517000e+00 -6.3662000e-01 -3.7382000e-01 /
CHEB / 6.6597000e+00 8.0784000e-01 4.5247000e-01 /
CHEB / 5.5885000e-01 -8.9071000e-02 -1.9526000e-02 /
CHEB / 2.6527000e-01 -9.6383000e-02 -6.0152000e-02 /
CHEB / 1.4478000e-01 -9.3242000e-03 -1.3861000e-02 /

aC3H5+O(+m)=C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -107.8488941989901
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / 7.5090000e+00 1.7654000e-02 1.0308000e-02 /
CHEB / 1.0312000e+00 -1.7426000e-02 -8.7674000e-03 /
CHEB / 2.6849000e-01 -4.9938000e-03 -5.3579000e-03 /
CHEB / 1.0834000e-01 4.6130000e-03 3.6393000e-03 /
CHEB / 4.2823000e-02 1.0719000e-03 9.3106000e-04 /

aC3H5+O(+m)=C3H5OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -74.58233610780096 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1748000e+00 -5.2774000e-03 -3.5367000e-03 /
CHEB / 8.9486000e-01 6.5859000e-03 4.3642000e-03 /
CHEB / 2.9334000e-01 -8.2727000e-04 -4.6906000e-04 /
CHEB / 1.1671000e-01 -5.3328000e-04 -3.9094000e-04 /
CHEB / 4.5235000e-02 -1.7767000e-05 -1.9650000e-05 /

aC3H5+O(+m)=CHCHCH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -72.38256073488924
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7215000e+00 -9.6721000e-04 -6.5038000e-04 /
CHEB / 8.7933000e-01 1.1618000e-03 7.7208000e-04 /
CHEB / 2.8449000e-01 -9.3616000e-05 -4.7758000e-05 /
CHEB / 1.1479000e-01 -1.0090000e-04 -7.3112000e-05 /
CHEB / 4.6344000e-02 -1.1934000e-05 -9.6597000e-06 /

aC3H5+O(+m)=C3H5OJ(17)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -79.4218978907725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3077000e+00 -2.5441000e-02 -1.7929000e-02 /
CHEB / 1.4804000e+00 3.2406000e-02 2.2949000e-02 /
CHEB / 4.7155000e-01 -5.3082000e-03 -3.9598000e-03 /
CHEB / 1.7661000e-01 -1.6852000e-03 -1.0672000e-03 /
CHEB / 5.9071000e-02 -1.7842000e-04 -1.1824000e-04 /

aC3H5+O(+m)=CH3CHcOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -80.0518545987924
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6364000e+00 -3.4922000e-02 -2.4615000e-02 /
CHEB / 1.2997000e+00 4.5495000e-02 3.2080000e-02 /
CHEB / 4.0162000e-01 -8.2099000e-03 -5.7878000e-03 /
CHEB / 1.4529000e-01 -3.0429000e-03 -2.1786000e-03 /
CHEB / 4.6346000e-02 2.5953000e-04 2.0570000e-04 /

pC3H5+O(+m)=C3H5OJ(8)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -131.31643615065116
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1096000e+01 1.0482000e-03 7.4875000e-04 /
CHEB / 3.6022000e-01 -1.3307000e-03 -9.5460000e-04 /
CHEB / 1.8057000e-01 1.9724000e-04 1.4734000e-04 /
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CHEB / 1.1353000e-01 8.3707000e-05 5.8284000e-05 /
CHEB / 5.5531000e-02 1.0570000e-05 6.3409000e-06 /

pC3H5+O(+m)=C3H5OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#3 (C3H5OJ(13))   deltaHrxn(T=298K) = -98.04987805946203 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1156000e+01 -7.2779000e-03 -5.2308000e-03 /
CHEB / -2.1609000e-01 9.1566000e-03 6.6203000e-03 /
CHEB / -4.0638000e-02 -1.4047000e-03 -1.0708000e-03 /
CHEB / 1.2887000e-02 -4.6484000e-04 -3.1699000e-04 /
CHEB / 9.9346000e-03 -6.7935000e-05 -4.1968000e-05 /

pC3H5+O(+m)=CHCHCH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -95.85010268655031
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0960000e+01 -7.0029000e-03 -5.0384000e-03 /
CHEB / -1.5041000e-01 8.8154000e-03 6.3813000e-03 /
CHEB / -2.5340000e-02 -1.3594000e-03 -1.0390000e-03 /
CHEB / 1.7919000e-02 -4.4232000e-04 -3.0111000e-04 /
CHEB / 1.1956000e-02 -6.6325000e-05 -4.0947000e-05 /

pC3H5+O(+m)=C3H5OJ(17)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -102.88943984243357
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1311000e+01 -2.2787000e-03 -1.6388000e-03 /
CHEB / 2.7976000e-01 2.7303000e-03 1.9777000e-03 /
CHEB / 9.1299000e-02 -2.3804000e-04 -1.9249000e-04 /
CHEB / 5.9544000e-02 -1.8452000e-04 -1.2801000e-04 /
CHEB / 3.0668000e-02 -4.3563000e-05 -2.8547000e-05 /

pC3H5+O(+m)=CH3CHcOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C3H5OJ(13))   deltaHrxn(T=298K) = -103.51939655045348
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1509000e+01 -3.2546000e-03 -2.3629000e-03 /
CHEB / 1.6468000e-01 4.1321000e-03 3.0228000e-03 /
CHEB / 4.9196000e-02 -6.7100000e-04 -5.2382000e-04 /
CHEB / 4.3049000e-02 -1.9510000e-04 -1.3063000e-04 /
CHEB / 2.3537000e-02 -3.3094000e-05 -2.0160000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown(1)        -34.2 84.51 21.22 25.67 29.58 32.47 37.32 40.64
      43.58 null
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
```

```
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     C2H4O+HCO=unknown(1)          5.2000000e+11      0.00000
6.5600000e+03
!     C3H4O+OH=unknown(1)           2.7100000e+12      0.00000
0.0000000e+00
!     C2H5O-1+CO=unknown(1)         4.0416992e+07      1.70125
8.2775000e+04

C2H4O+HCO(+m)=C2H5O-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown)      deltaHrxn(T=298K) = -13.188796045299238
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6087000e+01 3.5600000e-06 2.4789000e-06 /
CHEB / 2.4242000e+01 7.7101000e-07 5.3624000e-07 /
CHEB / 1.1065000e-01 -3.6927000e-07 -2.5745000e-07 /
CHEB / 3.2074000e-02 -2.7841000e-07 -1.9387000e-07 /
CHEB / -4.3799000e-03 -1.2774000e-07 -8.8866000e-08 /

C3H4O+OH(+m)=C2H4O+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown)      deltaHrxn(T=298K) = -13.52853992312419
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2451000e+01 -1.7966000e-01 -1.0658000e-01 /
CHEB / -1.7637000e-02 2.2288000e-01 1.2869000e-01 /
CHEB / -4.7704000e-02 -1.7403000e-02 -5.2598000e-03 /
CHEB / -3.7007000e-02 -2.8814000e-02 -1.7203000e-02 /
CHEB / -2.4170000e-02 -3.3181000e-03 -3.5883000e-03 /

C3H4O+OH(+m)=C2H5O-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown)      deltaHrxn(T=298K) = -26.717335968423427
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0443000e+01 -1.1100000e-04 -7.7309000e-05 /
CHEB / 1.9868000e+01 8.3372000e-05 5.8073000e-05 /
CHEB / 1.6263000e-01 3.3300000e-05 2.3191000e-05 /
CHEB / 4.8236000e-02 1.9537000e-06 1.3560000e-06 /
CHEB / 7.0932000e-04 -4.1482000e-06 -2.8911000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     aC3H5O2           24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67
      46.07
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     HO2         3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26 12.25
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+O2=aC3H5O2        2.2600000e+12      0.00000
0.0000000e+00
!     aC3H5O2=aC3H4+HO2       5.8013126e+10      0.62333
3.0055556e+04

aC3H5+O2(+m)=aC3H5O2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (aC3H5O2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     O2_birad       deltaHrxn(T=298K) = -
18.628026791741224 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7827000e+00 1.2538000e+00 -1.5048000e-01 /
CHEB / -3.8891000e+00 7.9488000e-01 1.3957000e-01 /
CHEB / -2.1985000e+00 9.8666000e-02 4.6089000e-02 /
CHEB / -1.0466000e+00 -9.9753000e-02 -1.5961000e-02 /
CHEB / -4.0790000e-01 -7.3246000e-02 -2.2284000e-02 /

aC3H4+HO2(+m)=aC3H5O2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (aC3H5O2)      deltaHrxn(T=298K) = -26.087213838026695
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3404000e+00 3.9220000e+00 5.6401000e-02 /
CHEB / -1.9502000e+00 2.0479000e-01 1.3322000e-01 /
CHEB / -2.0028000e+00 -7.3629000e-02 1.7058000e-02 /
CHEB / -9.4347000e-01 -1.2377000e-01 -2.6904000e-02 /
CHEB / -3.5909000e-01 -6.9799000e-02 -2.2673000e-02 /

aC3H4+HO2(+m)=aC3H5+O2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (aC3H5O2)      deltaHrxn(T=298K) = -7.459187046285471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4446000e+00 -4.7864000e-02 -3.6408000e-02 /
CHEB / 2.0709000e+00 6.2131000e-02 4.6932000e-02 /
CHEB / 2.3076000e-01 -7.9827000e-03 -5.5304000e-03 /
CHEB / 8.4331000e-02 -8.4057000e-03 -6.4953000e-03 /
CHEB / 2.8852000e-02 1.3407000e-04 -7.9108000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -80.3 83.37 22.52 26.92 30.64 33.84 39.43 43.34
      46.04 null
```

```
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H5OJ(13)        7.36  75.41 19.41 22.49 25.45 28.06 32.31 35.53
      40.59
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!Here are the path reactions and their high-P limit kinetics:
!     OH+C3H5OJ(13)=unknown1(1)     7.7000000e+13      0.00000
0.0000000e+00
!     CH2OH+CH2CHO=unknown1(1)      1.1500000e+13      0.00000
0.0000000e+00
!     C2H5O-1+HCO=unknown1(1)       1.8100000e+13      0.00000
0.0000000e+00
!     C2H5OH+CO=unknown1(1)         9.1400000e+04      2.53000
8.5500000e+04
!     H2O+C3H4O=unknown1(1)         2.2700000e+02      2.74000
5.6900000e+04

OH+C3H5OJ(13)(+m)=CH2OH+CH2CHO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -15.138089482203885
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2923000e+01 -8.2578000e-01 -1.9547000e-01 /
CHEB / 4.4302000e-01 8.2858000e-01 1.4084000e-01 /
CHEB / 3.6544000e-03 1.3827000e-01 8.7358000e-02 /
CHEB / -9.2122000e-02 -7.8945000e-02 3.7189000e-03 /
CHEB / -6.2193000e-02 -6.1538000e-02 -2.4506000e-02 /

OH+C3H5OJ(13)(+m)=C2H5O-1+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -11.758624205481022
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3272000e+01 -8.1301000e-01 -1.9080000e-01 /
CHEB / 4.9167000e-01 8.3290000e-01 1.4080000e-01 /
CHEB / 3.1687000e-02 1.2019000e-01 8.4949000e-02 /
CHEB / -8.7679000e-02 -8.5367000e-02 -1.7321000e-04 /
CHEB / -6.0791000e-02 -5.8397000e-02 -2.5378000e-02 /

OH+C3H5OJ(13)(+m)=C2H5OH+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -98.71948339151515
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0328000e+01 -8.1910000e-01 -1.9278000e-01 /
CHEB / 1.3613000e+00 8.3134000e-01 1.4075000e-01 /
CHEB / 2.5473000e-01 1.2852000e-01 8.6006000e-02 /
CHEB / -6.8292000e-03 -8.2679000e-02 1.5689000e-03 /
CHEB / -2.8811000e-02 -5.9946000e-02 -2.5020000e-02 /

OH+C3H5OJ(13)(+m)=H2O+C3H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -88.70081794717427
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0311000e+01 -8.4449000e-01 -2.1860000e-01 /
CHEB / 8.9404000e-01 7.9805000e-01 1.4571000e-01 /
CHEB / 1.0701000e-02 1.8177000e-01 9.7417000e-02 /
CHEB / -9.3752000e-02 -5.2792000e-02 1.6951000e-02 /
CHEB / -6.5429000e-02 -6.4392000e-02 -1.9966000e-02 /

CH2OH+CH2CHO(+m)=C2H5OH+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -83.58139390931127
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7058000e+00 -1.2470000e+00 -6.6746000e-02 /
CHEB / 3.3201000e+00 1.0684000e+00 -2.5888000e-02 /
CHEB / 2.4982000e-01 3.5785000e-01 7.1846000e-02 /
CHEB / -1.4140000e-01 -3.2982000e-02 4.9858000e-02 /
CHEB / -8.5600000e-02 -1.0038000e-01 -9.8086000e-04 /

CH2OH+CH2CHO(+m)=H2O+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -73.56272846497039
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8478000e+00 -1.3987000e+00 -4.2496000e-02 /
CHEB / 1.8498000e+00 9.6808000e-01 -3.8561000e-02 /
CHEB / 9.9641000e-02 4.8591000e-01 3.0963000e-02 /
CHEB / -2.2694000e-01 1.0312000e-01 4.6621000e-02 /
CHEB / -1.6462000e-01 -5.5594000e-02 2.0562000e-02 /

C2H5O-1+HCO(+m)=CH2OH+CH2CHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -3.3794652767228603
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1292000e+01 -1.2223000e+00 -7.3296000e-02 /
CHEB / 1.5473000e+00 1.0708000e+00 -2.0439000e-02 /
CHEB / 4.3416000e-02 3.3438000e-01 7.8075000e-02 /
CHEB / -1.8975000e-01 -4.5088000e-02 4.7857000e-02 /
CHEB / -1.0607000e-01 -9.9259000e-02 -4.3860000e-03 /

C2H5O-1+HCO(+m)=C2H5OH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -86.96085918603413
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 8.5625000e+00 -1.1973000e+00 -7.8798000e-02 /
CHEB / 2.5989000e+00 1.0743000e+00 -1.5105000e-02 /
CHEB / 2.7791000e-01 3.0963000e-01 8.3794000e-02 /
CHEB / -1.0348000e-01 -5.7983000e-02 4.5164000e-02 /
CHEB / -6.8641000e-02 -9.7977000e-02 -8.0149000e-03 /

C2H5O-1+HCO(+m)=H2O+C3H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -76.94219374169325
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3426000e+00 -1.3358000e+00 -5.7696000e-02 /
CHEB / 1.4970000e+00 1.0075000e+00 -3.5689000e-02 /
CHEB / 4.5282000e-02 4.3788000e-01 5.0504000e-02 /
CHEB / -1.9056000e-01 5.1949000e-02 5.2182000e-02 /
CHEB / -1.3328000e-01 -7.4321000e-02 1.4525000e-02 /

H2O+C3H4O(+m)=C2H5OH+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -10.018665444340886
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2423000e+01 -1.3655000e+00 -4.9986000e-02 /
CHEB / 2.8177000e+01 9.9218000e-01 -3.8074000e-02 /
CHEB / 2.6851000e-01 4.6151000e-01 4.1242000e-02 /
CHEB / -1.3811000e-01 7.4240000e-02 5.0239000e-02 /
CHEB / -1.1923000e-01 -6.7321000e-02 1.7603000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown(2)        -96.93      85.78 24.08 29.65 34.49 38.67 45.33
      50.22 53.79 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!Here are the path reactions and their high-P limit kinetics:
!     OH+C3H7O-N1=unknown(2)        7.7000000e+13      0.00000
0.0000000e+00
!     CH2OH+C2H5O-1=unknown(2)      1.1500000e+13      0.00000
0.0000000e+00
!     H2O+C3H6O-enol2=unknown(2)          2.2700000e+02      2.74000
5.6900000e+04
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OH+C3H7O-N1(+m)=CH2OH+C2H5O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown)      deltaHrxn(T=298K) = -7.349146599463811
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2648000e+01 -1.1340000e+00 -1.0226000e-01 /
CHEB / 1.2375000e+00 1.0669000e+00 5.6926000e-03 /
CHEB / 7.3355000e-02 2.6533000e-01 1.0075000e-01 /
CHEB / -1.5062000e-01 -8.3165000e-02 4.2088000e-02 /
CHEB / -9.8603000e-02 -1.0081000e-01 -1.7873000e-02 /

OH+C3H7O-N1(+m)=H2O+C3H6O-enol2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown)      deltaHrxn(T=298K) = -85.10153416255389
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1025000e+01 -1.2203000e+00 -9.7841000e-02 /
CHEB / 1.1982000e+00 1.0354000e+00 -1.4802000e-02 /
CHEB / -2.3887000e-02 3.5732000e-01 8.8703000e-02 /
CHEB / -1.7521000e-01 -1.6910000e-02 6.0995000e-02 /
CHEB / -1.2110000e-01 -9.8261000e-02 2.3908000e-03 /

CH2OH+C2H5O-1(+m)=H2O+C3H6O-enol2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (unknown) deltaHrxn(T=298K) = -77.75238756309008
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9806000e+00 -1.3633000e+00 -5.5170000e-02 /
CHEB / 1.5710000e+00 1.0070000e+00 -4.5513000e-02 /
CHEB / 5.3164000e-02 4.7930000e-01 4.4696000e-02 /
CHEB / -2.2634000e-01 7.1484000e-02 6.3266000e-02 /
CHEB / -1.6865000e-01 -8.7189000e-02 2.6554000e-02 /

!PDepNetwork C3H7-1 + C3H7-2
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+CH3=C3H7-1         9.6900000e+12      0.00000
9.0000000e+03
!     C3H6+H=C3H7-1           1.1800000e+13      0.00000
3.8000000e+03
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!     C3H7-2=C3H7-1                 2.9160000e+10      1.32000
4.0300000e+04
!     C3H6+H=C3H7-2           2.0100000e+13      0.00000
2.1000000e+03

C3H7-2(+m)=C3H7-1(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) High-P Limit: intra_H_migration exact:  Others-R2H_S
C_rad_out_H/NonDeC     Cs_H_out_2H        deltaHrxn(T=298K) = -
0.800047291313561 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3575000e+00 4.2006000e+00 -6.9895000e-01 /
CHEB / 1.0913000e+01 8.3456000e-01 -9.5744000e-03 /
CHEB / -1.8496000e+00 1.4444000e-01 5.9415000e-02 /
CHEB / -9.9784000e-01 -7.8565000e-02 3.1127000e-03 /
CHEB / -4.8523000e-01 -9.9887000e-02 -2.2195000e-02 /

C2H4+CH3(+m)=C3H7-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H2
C_methyl          deltaHrxn(T=298K) = -23.587292544682985 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5747000e+00 1.1761000e+00 -2.0378000e-01 /
CHEB / 6.7200000e-01 6.3972000e-01 1.5056000e-01 /
CHEB / -1.4459000e+00 2.1652000e-01 6.1788000e-02 /
CHEB / -7.5644000e-01 7.4581000e-03 8.1627000e-03 /
CHEB / -3.6805000e-01 -3.8464000e-02 -9.7210000e-03 /

C2H4+CH3(+m)=C3H7-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) deltaHrxn(T=298K) = -22.787245253369424 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9898000e+00 1.3973000e+00 -4.9699000e-01 /
CHEB / 4.1945000e+00 1.3819000e+00 1.4188000e-01 /
CHEB / -1.3970000e+00 3.2521000e-01 1.2575000e-01 /
CHEB / -8.0081000e-01 -4.3761000e-02 3.0919000e-02 /
CHEB / -4.0336000e-01 -9.0462000e-02 -1.1110000e-02 /

C3H6+H(+m)=C3H7-1(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H/Nd_Cd/H2
H_rad       deltaHrxn(T=298K) = -33.1262171061894 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9772000e+00 2.1284000e+00 -3.2537000e-01 /
CHEB / -1.0895000e+00 5.8705000e-01 1.9159000e-01 /
CHEB / -1.4038000e+00 2.2366000e-01 7.3516000e-02 /
CHEB / -7.2291000e-01 3.3841000e-02 7.1462000e-03 /
CHEB / -3.4559000e-01 -2.2149000e-02 -1.2492000e-02 /

C3H6+H(+m)=C3H7-2(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Cd/H/Nd
H_rad       deltaHrxn(T=298K) = -32.32616981487584 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1298000e+01 6.4478000e-01 -8.3728000e-02 /
CHEB / -1.4655000e+00 8.9141000e-01 -3.2659000e-02 /
CHEB / -1.4399000e+00 3.5457000e-01 5.2175000e-02 /
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CHEB / -8.2226000e-01 3.3339000e-02 4.1204000e-02 /
CHEB / -4.2240000e-01 -6.5675000e-02 4.4097000e-03 /

C3H6+H(+m)=C2H4+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7-1) deltaHrxn(T=298K) = -9.53892456150642 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1560000e+01 -3.4944000e-01 -1.6526000e-01 /
CHEB / 1.6856000e+00 3.7297000e-01 1.7084000e-01 /
CHEB / 1.2595000e-01 2.5194000e-02 1.7209000e-02 /
CHEB / 8.2871000e-04 -3.1039000e-02 -1.3374000e-02 /
CHEB / -2.4898000e-02 -1.1805000e-02 -5.2678000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown(1)        -52.3 88.58 23.81 28.97 33.53 37.01 42.82 46.98
      51.64 null
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     CH2OH+C2H4O =unknown(1)       2.4827386e+10      0.24400
1.0487500e+04
!     C3H6O-enol2+OH=unknown(1)           2.7100000e+12      0.00000
0.0000000e+00

C3H6O-enol2+OH(+m)=CH2OH+C2H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown)      deltaHrxn(T=298K) = -12.718346101727363
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0736000e+01 -1.1135000e+00 -8.5690000e-02 /
CHEB / 1.6763000e+00 1.1235000e+00 -1.9655000e-03 /
CHEB / -2.2883000e-01 2.2107000e-01 1.0427000e-01 /
CHEB / -2.0751000e-01 -1.3792000e-01 3.6325000e-02 /
CHEB / -6.7924000e-02 -1.1174000e-01 -2.8790000e-02 /

!PDepNetwork C3H7O2 + CH2CH2CH2OOH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H7O2            -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67
      54.73
!     CH2CH2CH2OOH      7.26  88.49 25.27 30.39 34.78 38.41 43.99 48.1
      54.53
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!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!     HO2         3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26 12.25
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+O2=C3H7O2        2.2600000e+12      0.00000
0.0000000e+00
!     C3H7O2=CH2CH2CH2OOH           1.5210000e+07      1.55000
2.1020000e+04
!     C3H7O2=C3H6+HO2         1.9160000e+08      1.46000
2.9400000e+04

CH2CH2CH2OOH(+m)=C3H7O2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O2) deltaHrxn(T=298K) = -15.638097165645299 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4264000e+00 1.1857000e+00 -1.5567000e-01 /
CHEB / -3.9133000e+00 9.5956000e-01 6.8837000e-02 /
CHEB / -3.4133000e+00 -1.4953000e-01 4.6845000e-02 /
CHEB / -1.6062000e+00 -2.4841000e-01 -7.4833000e-02 /
CHEB / -6.1152000e-01 -5.0727000e-02 -4.6108000e-02 /

CH2CH2CH2OOH(+m)=C3H6+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O2) deltaHrxn(T=298K) = 2.0500177010023215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3504000e-01 4.4336000e-01 -3.0100000e-01 /
CHEB / 1.5549000e+00 1.4640000e+00 3.0712000e-01 /
CHEB / -2.4975000e+00 2.6317000e-02 1.9470000e-02 /
CHEB / -1.3587000e+00 -7.3978000e-02 -1.1442000e-01 /
CHEB / -6.0321000e-01 3.4183000e-02 -1.1488000e-02 /

C3H7-1+O2(+m)=C3H7O2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O2) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cs     O2_birad       deltaHrxn(T=298K) = -
34.26632664092392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0172000e+01 9.2348000e-01 -1.2686000e-01 /
CHEB / -4.1410000e+00 1.2507000e+00 -7.8379000e-02 /
CHEB / -2.7986000e+00 4.8139000e-01 2.8677000e-02 /
CHEB / -1.6152000e+00 3.0427000e-02 2.7312000e-02 /
CHEB / -7.7073000e-01 -1.0347000e-01 -2.4494000e-03 /

C3H7-1+O2(+m)=CH2CH2CH2OOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O2) deltaHrxn(T=298K) = -18.628229475278626 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4213000e+00 9.6073000e-01 -3.9990000e-01 /
CHEB / -4.3566000e+00 1.5664000e+00 3.2626000e-01 /
CHEB / -2.8102000e+00 3.8903000e-02 -1.2822000e-02 /
CHEB / -1.4384000e+00 -6.4036000e-02 -1.2312000e-01 /
CHEB / -6.3221000e-01 4.6470000e-02 -5.3453000e-03 /
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C3H7-1+O2(+m)=C3H6+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H7O2) deltaHrxn(T=298K) = -16.578211774276305 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9516000e+00 -1.0143000e+00 -1.1366000e-01 /
CHEB / 4.8378000e-01 1.0174000e+00 2.5185000e-02 /
CHEB / -7.0976000e-01 1.3821000e-01 8.0386000e-02 /
CHEB / -6.3966000e-01 -1.1934000e-01 1.6027000e-02 /
CHEB / -3.8366000e-01 -7.7197000e-02 -1.8458000e-02 /

C3H6+HO2(+m)=C3H7O2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C3H7O2) deltaHrxn(T=298K) = -17.688114866647616 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9716000e+00 5.9558000e-01 -4.3369000e-02 /
CHEB / 1.6455000e+00 9.4394000e-01 -4.5489000e-02 /
CHEB / -2.1986000e+00 4.4316000e-01 1.6660000e-02 /
CHEB / -1.4191000e+00 5.1760000e-02 2.9662000e-02 /
CHEB / -7.0331000e-01 -9.9123000e-02 6.0019000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -101.3      85.17 24.58 30.33 35.44 39.41 45.98
      50.72 56.3  null
!     C3H6O-enol        -34.7 70.85 20.67 24.56 28.02 30.98 35.68 39.25
      45.02
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol+H2O=unknown1(1)          1.1691492e+02      2.87714
4.8857143e+04
!     H2O+H2CCCH3[OH]=unknown1(1)         1.1691492e+02      2.87714
4.8857143e+04
!     C3H6O-enol2+H2O=unknown1(1)         6.5200000e+01      2.92000
5.0700000e+04
!     CH3OH+C2H4O=unknown1(1)       1.6297242e+02      2.92024
4.4628571e+04

C3H6O-enol+H2O(+m)=H2O+H2CCCH3[OH](+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
4.73945625358796 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4786000e+01 -1.5090000e+00 -3.7819000e-02 /
CHEB / 2.2419000e+01 8.7078000e-01 -5.3203000e-02 /
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CHEB / 8.9898000e-01 5.9070000e-01 -2.5512000e-03 /
CHEB / -1.5060000e-01 2.6602000e-01 4.0844000e-02 /
CHEB / -2.4465000e-01 1.4806000e-02 5.2036000e-02 /

C3H6O-enol2+H2O(+m)=C3H6O-enol+H2O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
5.769265895614019 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5677000e+01 -1.4753000e+00 -4.1135000e-02 /
CHEB / 2.2668000e+01 9.1435000e-01 -5.3729000e-02 /
CHEB / 8.3986000e-01 5.8343000e-01 7.7156000e-03 /
CHEB / -1.3810000e-01 2.2210000e-01 5.3205000e-02 /
CHEB / -2.1039000e-01 -2.8441000e-02 5.3869000e-02 /

C3H6O-enol2+H2O(+m)=H2O+H2CCCH3[OH](+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
10.508722149201986 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4917000e+01 -1.4855000e+00 -4.0228000e-02 /
CHEB / 2.2253000e+01 9.0165000e-01 -5.3800000e-02 /
CHEB / 8.1410000e-01 5.8687000e-01 4.4241000e-03 /
CHEB / -1.2933000e-01 2.3648000e-01 4.9575000e-02 /
CHEB / -2.1622000e-01 -1.5524000e-02 5.3765000e-02 /

CH3OH+C2H4O(+m)=C3H6O-enol+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -15.568917049355967
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2303000e+01 -1.4647000e+00 -4.2416000e-02 /
CHEB / 2.0113000e+01 9.2727000e-01 -5.4036000e-02 /
CHEB / 7.9491000e-01 5.7946000e-01 1.1201000e-02 /
CHEB / -1.5547000e-01 2.0738000e-01 5.7149000e-02 /
CHEB / -2.1012000e-01 -4.0970000e-02 5.4147000e-02 /

CH3OH+C2H4O(+m)=H2O+H2CCCH3[OH](+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -20.308373302943934
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1609000e+01 -1.4742000e+00 -4.1571000e-02 /
CHEB / 1.9767000e+01 9.1584000e-01 -5.4161000e-02 /
CHEB / 7.5890000e-01 5.8351000e-01 8.0712000e-03 /
CHEB / -1.4977000e-01 2.2130000e-01 5.3900000e-02 /
CHEB / -2.1525000e-01 -2.9362000e-02 5.4328000e-02 /

CH3OH+C2H4O(+m)=C3H6O-enol2+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -9.799651153741948
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3772000e+01 -1.4468000e+00 -4.4290000e-02 /
CHEB / 2.1186000e+01 9.4830000e-01 -5.4072000e-02 /
CHEB / 8.9282000e-01 5.7077000e-01 1.7104000e-02 /
CHEB / -1.3944000e-01 1.8107000e-01 6.3062000e-02 /
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CHEB / -1.8724000e-01 -6.1373000e-02 5.3578000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+CH2CHO=unknown2(2) 1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+HCO=unknown2(2)         1.4157154e+13      -0.15000
2.9166667e+02
!     C3H6+CO=unknown2(2)           9.1400000e+04      2.53000
8.5500000e+04

C2H3+CH2CHO(+m)=aC3H5+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (unknown2)     deltaHrxn(T=298K) = -24.827514103787152
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2568000e+01 -3.2770000e-01 -1.7826000e-01 /
CHEB / 4.4987000e-02 3.3648000e-01 1.7507000e-01 /
CHEB / -3.6489000e-02 5.4049000e-02 3.6380000e-02 /
CHEB / -5.7155000e-02 -4.1910000e-02 -1.7949000e-02 /
CHEB / -4.7296000e-02 -2.5551000e-02 -1.5462000e-02 /

C2H3+CH2CHO(+m)=C3H6+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (unknown2)     deltaHrxn(T=298K) = -97.14014475820552
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9658000e+00 -3.4135000e-01 -1.6961000e-01 /
CHEB / 1.8373000e+00 3.7328000e-01 1.7582000e-01 /
CHEB / 5.1259000e-01 2.9415000e-02 2.5133000e-02 /
CHEB / 1.0878000e-01 -4.9645000e-02 -2.1004000e-02 /
CHEB / 7.5455000e-03 -1.9635000e-02 -1.2913000e-02 /

aC3H5+HCO(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (unknown2)     deltaHrxn(T=298K) = -72.31263065441836
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2063000e+00 -8.1291000e-01 -1.9937000e-01 /
CHEB / 5.8901000e+00 8.0205000e-01 1.4563000e-01 /
CHEB / 2.6839000e-01 1.4946000e-01 8.3086000e-02 /
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CHEB / -1.0805000e-02 -7.4488000e-02 6.5226000e-03 /
CHEB / -3.8563000e-02 -6.0682000e-02 -2.2452000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -58.15      88.45 25.06 30.58 35.41 39.08 45.18
      49.33 53.47 null
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     C3H5O-enol2+HCO=unknown3(3)   1.4157154e+13      -0.15000
2.9166667e+02
!     C3H6O-enol2+CO=unknown3(3)          7.6600000e+05      2.07000
8.2200000e+04

C3H5O-enol2+HCO(+m)=C3H6O-enol2+CO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #17 (unknown3)     deltaHrxn(T=298K) = -
64.06384844315242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8101000e+00 -9.3062000e-01 -1.8658000e-01 /
CHEB / 7.6037000e+00 8.9539000e-01 1.0384000e-01 /
CHEB / 2.5116000e-01 1.9120000e-01 1.0686000e-01 /
CHEB / -1.5699000e-02 -6.8262000e-02 2.3265000e-02 /
CHEB / -3.9183000e-02 -7.5215000e-02 -2.3988000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       -125.08     119.3 35.57 47.41 54.44 59.72 67.62
      72.56 76.88 null
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(801)+nSPC(543)=unknown4(4)     1.4157154e+13      -0.15000
2.9166667e+02
!     nSPC(879)+CH2CHO=unknown4(4)  1.4157154e+13      -0.15000
2.9166667e+02
```

```
nSPC(801)+nSPC(543)(+m)=nSPC(879)+CH2CHO(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #48 (unknown4)    deltaHrxn(T=298K)
= -7.988646506677688 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6493000e+00 -1.5353000e-01 -9.0222000e-02 /
CHEB / 2.0087000e+00 1.9076000e-01 1.0948000e-01 /
CHEB / 5.2872000e-01 -1.5766000e-02 -5.4023000e-03 /
CHEB / 8.1087000e-02 -2.5305000e-02 -1.5100000e-02 /
CHEB / -4.2227000e-03 -9.4698000e-04 -1.8902000e-03 /

!PDepNetwork C4H7OJ(8) + C4H7OJ(12) + C4H7OJ(13) + C4H7OJ(16)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(16)        -0.43 85.56 24.15 29.0  33.26 36.92 43.23 47.77
      53.44 null
!     C4H7OJ(8)         -12.53      83.27 24.09 28.93 33.21 36.9  43.23
      47.78 53.46 null
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     C4H7OJ(13)        -2.61 86.64 23.05 27.77 32.28 36.23 42.54 47.26
      54.54  !MRH CBS-QB3 w/1DHR corrections
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH2CO       -10.78      57.63 12.31 14.11 15.57 16.77 18.67 20.12
      22.44
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     CH3CHCHCHO        -28.19      75.98 22.26 27.43 31.78 35.41 41.16
      45.23 50.19 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     C4H7-11           58.99 75.0  20.38 25.34 29.68 33.36 39.14 43.48
      50.22 null
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C2H4+CH2CHO=C4H7OJ(16)  2.4827386e+10      0.24400
9.0875000e+03
```

```
!     C3H7-1+CO=C4H7OJ(16)    9.1400000e+04      2.53000
8.5500000e+04
!     C4H7OJ(16)=C4H7OJ(8)          2.0320555e+08      1.13906
3.4790987e+04
!     C2H5+CH2CO=C4H7OJ(8)    1.9263655e+11      0.04067
9.2900000e+03
!     C4H7OJ(12)=C4H7OJ(8)          2.0320555e+08      1.13906
3.4790987e+04
!     CH3+C3H4O=C4H7OJ(12)    7.3000000e+12      0.00000
5.7000000e+03
!     CH3CHCHCHO+H=C4H7OJ(12)       1.0000000e+13      0.00000
2.9000000e+03
!     C4H7OJ(13)=C4H7OJ(12)         3.3640000e+10      0.35000
2.9900000e+04
!     C3H6+HCO=C4H7OJ(13)     5.2000000e+11      0.00000
6.5600000e+03
!     CH3CHCHCHO+H=C4H7OJ(13)       2.8500000e+13      0.00000
4.3000000e+03
!     C3H7-2+CO=C4H7OJ(13)    4.0416992e+07      1.70125
8.2775000e+04
!     C4H7OJ(16)=C4H7OJ(13)         3.8760000e+10      0.89000
3.5800000e+04
!     C4H7OJ(13)=C4H7OJ(8)          2.0320555e+08      1.13906
3.4790987e+04
!     C4H7OJ(16)=C4H7OJ(12)         6.6400000e+08      1.10000
2.9400000e+04
!     C4H7-11+O=C4H7OJ(12)    1.0000000e+13      0.00000
0.0000000e+00
!     C3H7-1+CO=C4H7OJ(8)     1.5100000e+11      0.00000
4.8100000e+03

C4H7OJ(16)(+m)=C4H7OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration estimate:
(Average:) R4H_SSS     C_rad_out_2H     CO_H_out      deltaHrxn(T=298K)
= -12.098773974071525 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8236000e+01 7.1982000e+00 8.3808000e-01 /
CHEB / 8.0078000e+00 -1.7477000e-01 -2.0000000e-01 /
CHEB / -2.4191000e+00 -7.9281000e-01 -3.4596000e-02 /
CHEB / -1.3844000e+00 -3.7587000e-01 4.9785000e-02 /
CHEB / -6.7694000e-01 -1.1172000e-01 6.0028000e-02 /

C4H7OJ(16)(+m)=C4H7OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration exact:
Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -5.909161961689662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.4668000e+00 2.5428000e+00 -6.1231000e-01 /
CHEB / 4.1072000e+00 2.0913000e+00 1.9225000e-02 /
CHEB / -3.7105000e+00 2.9761000e-01 2.2833000e-01 /
CHEB / -1.9619000e+00 -3.1709000e-01 9.8076000e-02 /
CHEB / -8.4358000e-01 -3.1926000e-01 -1.4496000e-02 /

C4H7OJ(16)(+m)=C4H7OJ(13)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration exact:
```

```
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.179560236367433 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8797000e+00 2.6835000e+00 -3.3906000e-01 /
CHEB / 7.3032000e+00 1.6850000e+00 -6.2330000e-02 /
CHEB / -2.7643000e+00 -5.0695000e-02 7.9880000e-02 /
CHEB / -1.6167000e+00 -2.6553000e-01 3.2890000e-02 /
CHEB / -7.9242000e-01 -2.5330000e-01 -3.6757000e-02 /

C4H7OJ(16)(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -0.7998805062949543
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5210000e+00 9.9283000e-01 -1.7260000e-01 /
CHEB / 9.1514000e+00 1.2409000e+00 -3.4932000e-02 /
CHEB / -2.0126000e+00 4.8704000e-01 8.6073000e-02 /
CHEB / -1.2648000e+00 4.2548000e-02 6.6792000e-02 /
CHEB / -6.7817000e-01 -1.1872000e-01 1.0928000e-02 /

C4H7OJ(16)(+m)=C3H7-2+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = 1.6678501860667438E-4
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4479000e+01 1.1428000e+01 -1.0402000e+00 /
CHEB / 2.4834000e+01 -8.7903000e-01 1.1767000e+00 /
CHEB / -2.6895000e+00 -7.2222000e-01 6.0525000e-01 /
CHEB / -1.5580000e+00 -4.3608000e-01 1.4959000e-01 /
CHEB / -8.4002000e-01 -1.4933000e-01 -4.7826000e-02 /

C4H7OJ(12)(+m)=C4H7OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_H/NonDeC     CO_H_out
      deltaHrxn(T=298K) = -6.189612012381863 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7657000e+01 8.3826000e+00 -7.9078000e-02 /
CHEB / 6.2112000e+00 2.9914000e-01 -8.7771000e-02 /
CHEB / -3.5007000e+00 -5.8398000e-01 1.8760000e-01 /
CHEB / -1.7522000e+00 -4.1037000e-01 6.7708000e-02 /
CHEB / -7.4422000e-01 -5.5286000e-02 -3.4656000e-02 /

C4H7OJ(13)(+m)=C4H7OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    C_rad_out_H/NonDeC     CO_H_out
      deltaHrxn(T=298K) = -9.919213737704093 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8688000e+01 8.6683000e+00 2.9364000e-01 /
CHEB / 8.2565000e+00 -6.8670000e-01 -1.3382000e-01 /
CHEB / -2.3568000e+00 -1.0329000e+00 9.2890000e-02 /
CHEB / -1.3098000e+00 -4.4467000e-01 4.4447000e-02 /
CHEB / -6.3058000e-01 -7.0174000e-02 2.8978000e-02 /
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C4H7OJ(13)(+m)=C4H7OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_H/NonDeC     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -3.7296017253222296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4774000e+00 3.0043000e+00 -8.4510000e-01 /
CHEB / 4.0677000e+00 1.8234000e+00 1.0504000e-01 /
CHEB / -3.7163000e+00 2.0477000e-01 2.1455000e-01 /
CHEB / -1.8922000e+00 -3.5100000e-01 7.6831000e-02 /
CHEB / -7.7250000e-01 -3.0991000e-01 -2.1173000e-02 /

C4H7OJ(13)(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = 1.3796797300724783
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1009000e+00 2.6435000e+00 -5.2599000e-01 /
CHEB / 8.9629000e+00 6.8983000e-01 2.6584000e-01 /
CHEB / -1.9426000e+00 1.6107000e-01 1.2835000e-01 /
CHEB / -1.0810000e+00 -7.1633000e-02 8.3335000e-03 /
CHEB / -5.1403000e-01 -1.1044000e-01 -1.9810000e-02 /

C4H7OJ(13)(+m)=C3H7-2+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = 2.1797270213860394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9730000e+01 1.2581000e+01 -1.2931000e-01 /
CHEB / 2.6767000e+01 -5.0740000e-01 3.1323000e-01 /
CHEB / -2.1499000e+00 -9.1809000e-01 5.8952000e-01 /
CHEB / -1.2459000e+00 -6.8985000e-01 2.7722000e-01 /
CHEB / -6.4201000e-01 -3.6790000e-01 7.7153000e-02 /

C2H4+CH2CHO(+m)=C4H7OJ(16)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H2     C_rad/H2/CO      deltaHrxn(T=298K)
= -18.72840807354501 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9110000e+00 5.9389000e-01 -5.1149000e-02 /
CHEB / 5.1346000e-01 9.2973000e-01 -3.5420000e-02 /
CHEB / -1.9459000e+00 4.4177000e-01 4.4812000e-02 /
CHEB / -1.2502000e+00 6.0834000e-02 5.4772000e-02 /
CHEB / -6.8759000e-01 -1.0517000e-01 1.6142000e-02 /

C2H4+CH2CHO(+m)=C4H7OJ(8)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -30.827182047616535
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2903000e+01 5.8394000e+00 9.1908000e-01 /
CHEB / 4.1979000e+00 2.5380000e-01 -2.0226000e-01 /
CHEB / -1.3733000e+00 -3.9607000e-01 1.4099000e-02 /
CHEB / -9.3846000e-01 -3.0366000e-01 1.0965000e-01 /
CHEB / -5.4762000e-01 -1.5161000e-01 1.0829000e-01 /
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C2H4+CH2CHO(+m)=C4H7OJ(12)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -24.637570035234674
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7755000e-01 1.4379000e+00 -6.4824000e-01 /
CHEB / 5.5373000e-01 2.8633000e+00 8.9071000e-02 /
CHEB / -2.7556000e+00 5.1093000e-01 2.7921000e-01 /
CHEB / -1.6351000e+00 -2.0450000e-01 1.3151000e-01 /
CHEB / -7.5288000e-01 -2.4809000e-01 1.7658000e-02 /

C2H4+CH2CHO(+m)=C4H7OJ(13)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -20.90796830991244
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.7476000e-01 1.8590000e+00 -4.2751000e-01 /
CHEB / 3.6349000e+00 1.9326000e+00 6.8215000e-02 /
CHEB / -1.7239000e+00 1.7662000e-01 1.7208000e-01 /
CHEB / -1.1967000e+00 -1.1002000e-01 3.1188000e-02 /
CHEB / -6.3817000e-01 -1.6373000e-01 -2.0748000e-02 /

C2H4+CH2CHO(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -19.528288579839963
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4429000e+00 -1.0527000e+00 -1.4048000e-01 /
CHEB / 6.9958000e+00 1.0045000e+00 4.4770000e-02 /
CHEB / 1.1729000e-01 2.3550000e-01 1.1361000e-01 /
CHEB / -1.5656000e-01 -6.9978000e-02 3.9023000e-02 /
CHEB / -9.3203000e-02 -9.3612000e-02 -2.1952000e-02 /

C2H4+CH2CHO(+m)=C2H5+CH2CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = 0.3496943904610923
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0781000e+00 -9.3285000e-01 -1.6218000e-01 /
CHEB / 8.6643000e+00 9.7638000e-01 8.5160000e-02 /
CHEB / 5.8974000e-01 1.2766000e-01 1.1703000e-01 /
CHEB / -4.5832000e-03 -1.0360000e-01 1.1429000e-02 /
CHEB / -2.9633000e-02 -7.5003000e-02 -3.5059000e-02 /

C2H4+CH2CHO(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -1.9799500725532493
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4308000e+00 -1.2241000e+00 -2.6514000e-01 /
CHEB / 7.1667000e+00 1.2428000e+00 1.9579000e-01 /
CHEB / -4.8023000e-02 1.8441000e-01 1.1037000e-01 /
CHEB / -2.7201000e-01 -9.6567000e-02 1.3334000e-02 /
CHEB / -1.5726000e-01 -9.1456000e-02 -2.5303000e-02 /
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C2H4+CH2CHO(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -18.7282412885264
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5967000e+01 -4.1814000e-02 -3.4981000e-02 /
CHEB / 2.3107000e+01 5.1587000e-02 4.2563000e-02 /
CHEB / 1.5430000e-01 -6.7698000e-04 1.4973000e-04 /
CHEB / -6.6540000e-03 -1.0571000e-02 -8.6753000e-03 /
CHEB / -2.3051000e-02 -1.9378000e-03 -1.8779000e-03 /

C3H7-1+CO(+m)=C4H7OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_COm exact:
C_rad/H2/Cs     COm           deltaHrxn(T=298K) = -11.298893467776573
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0131000e+00 1.4665000e+00 -1.6439000e-01 /
CHEB / -2.7393000e+00 5.9344000e-01 1.7909000e-01 /
CHEB / -2.4632000e+00 5.9579000e-02 2.2454000e-02 /
CHEB / -1.1143000e+00 -9.7958000e-02 -2.7117000e-02 /
CHEB / -4.0343000e-01 -5.6523000e-02 -2.0229000e-02 /

C3H7-1+CO(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -5.10928145539471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4368000e+00 2.4511000e+00 -5.5834000e-01 /
CHEB / 5.7208000e+00 2.1123000e+00 5.4724000e-02 /
CHEB / -2.7782000e+00 4.0347000e-01 2.5186000e-01 /
CHEB / -1.4171000e+00 -1.8600000e-01 1.1936000e-01 /
CHEB / -5.7950000e-01 -2.0167000e-01 9.1960000e-03 /

C2H5+CH2CO(+m)=C4H7OJ(16)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -19.0781024640061
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9280000e+00 1.4248000e+00 -2.2950000e-01 /
CHEB / 4.1258000e+00 1.7078000e+00 -1.2089000e-02 /
CHEB / -1.7181000e+00 5.8645000e-01 1.3520000e-01 /
CHEB / -1.2513000e+00 7.1084000e-03 8.4652000e-02 /
CHEB / -6.9433000e-01 -1.5029000e-01 4.0475000e-03 /

C2H5+CH2CO(+m)=C4H7OJ(8)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_rad/H2/Cs     Cd/H2_Ck         deltaHrxn(T=298K)
= -31.176876438077628 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3046000e+00 6.7408000e+00 6.1693000e-01 /
CHEB / 1.4178000e-01 -9.2181000e-01 4.5129000e-02 /
CHEB / -1.9157000e+00 -7.4612000e-01 6.8496000e-02 /
CHEB / -9.9093000e-01 -2.5215000e-01 1.5914000e-02 /
CHEB / -4.9894000e-01 7.1761000e-02 -3.2251000e-03 /
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C2H5+CH2CO(+m)=C4H7OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -24.987264425695763
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7624000e+00 3.2818000e+00 -6.3325000e-01 /
CHEB / 3.2145000e-01 2.5491000e+00 1.4635000e-01 /
CHEB / -2.5421000e+00 3.7644000e-01 2.7243000e-01 /
CHEB / -1.3567000e+00 -2.1635000e-01 1.0574000e-01 /
CHEB / -5.8202000e-01 -2.0403000e-01 1.2260000e-02 /

C2H5+CH2CO(+m)=C4H7OJ(13)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -21.257662700373537
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9987000e+00 3.2253000e+00 -4.7325000e-01 /
CHEB / 3.0701000e+00 1.1560000e+00 3.5083000e-01 /
CHEB / -1.5737000e+00 2.2801000e-01 1.1502000e-01 /
CHEB / -9.6394000e-01 -1.0864000e-01 3.7904000e-03 /
CHEB / -4.7618000e-01 -1.1773000e-01 -2.4694000e-02 /

C2H5+CH2CO(+m)=C3H6+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -2.3296444630143416
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0730000e-01 -2.8453000e-01 -1.4933000e-01 /
CHEB / 7.6105000e+00 3.5379000e-01 1.7570000e-01 /
CHEB / 8.4050000e-01 -3.3524000e-02 -2.1477000e-03 /
CHEB / 1.9659000e-01 -4.0253000e-02 -2.3284000e-02 /
CHEB / 4.5114000e-02 -2.3327000e-03 -5.7809000e-03 /

C2H5+CH2CO(+m)=C3H7-2+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -19.077935678987494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8842000e+01 -6.5390000e-03 -4.4347000e-03 /
CHEB / 2.4103000e+01 3.7246000e-03 2.4613000e-03 /
CHEB / 7.8142000e-01 3.9359000e-03 2.7013000e-03 /
CHEB / 2.7479000e-01 3.1611000e-04 2.8387000e-04 /
CHEB / 8.1363000e-02 -1.0996000e-03 -7.5081000e-04 /

CH3+C3H4O(+m)=C4H7OJ(16)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -21.477599726507876
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4322000e+00 1.4858000e-01 -2.6313000e-01 /
CHEB / 1.2773000e+00 1.9154000e+00 8.9256000e-02 /
CHEB / -1.9302000e+00 4.9060000e-01 9.0250000e-02 /
CHEB / -1.3034000e+00 -4.8357000e-03 2.5691000e-02 /
CHEB / -6.9206000e-01 -1.1232000e-01 -4.0578000e-03 /
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CH3+C3H4O(+m)=C4H7OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -33.5763737005794
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7630000e+00 6.0360000e+00 4.8659000e-01 /
CHEB / 5.2362000e-01 2.5679000e-01 2.2374000e-01 /
CHEB / -1.7721000e+00 -5.1414000e-01 1.7864000e-01 /
CHEB / -1.0177000e+00 -3.5048000e-01 4.3477000e-02 /
CHEB / -5.1073000e-01 -5.1747000e-02 -8.1771000e-03 /

CH3+C3H4O(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond exact:
C_methyl     Cd/H2_Cd/H/De          deltaHrxn(T=298K) = -
27.386761688197538 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0430000e+00 2.2268000e+00 -5.0888000e-01 /
CHEB / -3.5096000e+00 2.0528000e+00 4.2926000e-04 /
CHEB / -3.1680000e+00 3.8853000e-01 2.3208000e-01 /
CHEB / -1.5598000e+00 -1.9753000e-01 1.1489000e-01 /
CHEB / -6.3179000e-01 -2.0841000e-01 7.7614000e-03 /

CH3+C3H4O(+m)=C4H7OJ(13)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -23.657159962875312
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5057000e+00 1.2978000e+00 -5.1728000e-01 /
CHEB / -4.9721000e-02 2.0314000e+00 2.8001000e-01 /
CHEB / -2.0103000e+00 3.2150000e-01 1.4783000e-01 /
CHEB / -1.1401000e+00 -1.2283000e-01 1.3319000e-02 /
CHEB / -5.2565000e-01 -1.1918000e-01 -2.7373000e-02 /

CH3+C3H4O(+m)=C2H4+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -2.7491916529628684
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5917000e+00 -1.5800000e+00 -2.5066000e-01 /
CHEB / 5.0107000e+00 1.6293000e+00 1.7383000e-01 /
CHEB / -1.2872000e-01 1.8690000e-01 1.0795000e-01 /
CHEB / -2.7007000e-01 -1.0932000e-01 2.1285000e-02 /
CHEB / -1.2413000e-01 -9.8274000e-02 -1.6581000e-02 /

CH3+C3H4O(+m)=C3H6+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -4.729141725516117
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1479000e+00 -1.0768000e+00 -3.1819000e-01 /
CHEB / 3.8510000e+00 1.2892000e+00 3.1613000e-01 /
CHEB / 1.2244000e-01 -6.9194000e-02 7.1777000e-02 /
CHEB / -6.6355000e-03 -1.3254000e-01 -4.5494000e-02 /
CHEB / 1.0894000e-02 -3.1080000e-02 -2.9981000e-02 /
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```
CH3+C3H4O(+m)=C3H7-2+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -21.47743294148927
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4512000e+01 -3.6105000e-03 -2.9285000e-03 /
CHEB / 2.2280000e+01 2.2942000e-03 1.7588000e-03 /
CHEB / 3.8503000e-01 3.0906000e-03 2.5966000e-03 /
CHEB / 1.2291000e-01 -6.8556000e-04 -4.7733000e-04 /
CHEB / 2.4192000e-02 -1.6484000e-03 -1.3714000e-03 /

CH3CHCHCHO+H(+m)=C4H7OJ(16)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -24.337136418237957
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6559000e+00 1.8201000e-01 -2.4773000e-01 /
CHEB / 6.9088000e-01 2.0362000e+00 9.4096000e-02 /
CHEB / -1.8144000e+00 5.5499000e-01 9.8043000e-02 /
CHEB / -1.2450000e+00 1.9798000e-02 2.4823000e-02 /
CHEB / -6.6045000e-01 -1.1146000e-01 -8.5740000e-03 /

CH3CHCHCHO+H(+m)=C4H7OJ(8)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -36.43591039230948
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.4505000e+00 6.0628000e+00 4.7509000e-01 /
CHEB / 1.3538000e-01 2.4923000e-01 2.2975000e-01 /
CHEB / -1.5364000e+00 -5.0991000e-01 1.7814000e-01 /
CHEB / -8.4483000e-01 -3.5684000e-01 4.1170000e-02 /
CHEB / -3.9489000e-01 -7.3187000e-02 -6.1743000e-03 /

CH3CHCHCHO+H(+m)=C4H7OJ(12)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/De     H_rad        deltaHrxn(T=298K)
= -30.246298379927623 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3287000e+00 2.1338000e+00 -4.8058000e-01 /
CHEB / -4.3003000e+00 2.0518000e+00 -2.3156000e-02 /
CHEB / -3.1317000e+00 4.0501000e-01 2.2485000e-01 /
CHEB / -1.5446000e+00 -1.8748000e-01 1.1510000e-01 /
CHEB / -6.1596000e-01 -2.0472000e-01 8.7010000e-03 /

CH3CHCHCHO+H(+m)=C4H7OJ(13)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/De_Cd/H/Nd     H_rad        deltaHrxn(T=298K)
= -26.51669665460539 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3483000e+00 1.5707000e+00 -3.2997000e-01 /
CHEB / -1.7522000e+00 8.8302000e-01 1.8763000e-01 /
CHEB / -2.0158000e+00 2.5796000e-01 8.7326000e-02 /
CHEB / -1.0705000e+00 -6.1343000e-02 1.6291000e-02 /
CHEB / -4.9899000e-01 -1.0928000e-01 -1.6366000e-02 /
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CH3CHCHCHO+H(+m)=C2H4+CH2CHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -5.60872834469295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9208000e+00 -1.5805000e+00 -2.4567000e-01 /
CHEB / 4.6834000e+00 1.6521000e+00 1.7301000e-01 /
CHEB / 1.4054000e-01 1.7580000e-01 1.0703000e-01 /
CHEB / -1.3499000e-01 -1.2619000e-01 1.7449000e-02 /
CHEB / -6.8244000e-02 -1.0592000e-01 -1.8677000e-02 /

CH3CHCHCHO+H(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -25.13701692453291
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2842000e+00 -6.3297000e-01 -1.6354000e-01 /
CHEB / 3.9931000e+00 7.7517000e-01 1.5793000e-01 /
CHEB / 5.7837000e-01 -5.6343000e-02 4.8428000e-02 /
CHEB / 1.6532000e-01 -9.3101000e-02 -3.1084000e-02 /
CHEB / 5.3022000e-02 -9.2740000e-03 -1.8567000e-02 /

CH3CHCHCHO+H(+m)=C2H5+CH2CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -5.259033954231857
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3048000e+00 -4.3014000e-01 -1.5516000e-01 /
CHEB / 6.2065000e+00 5.6742000e-01 1.8000000e-01 /
CHEB / 1.0675000e+00 -1.0597000e-01 3.8804000e-03 /
CHEB / 2.8502000e-01 -4.6729000e-02 -3.1030000e-02 /
CHEB / 7.4256000e-02 1.0525000e-02 -2.9514000e-03 /

CH3CHCHCHO+H(+m)=CH3+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -2.8595366917300797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1003000e+01 -6.8565000e-01 -1.6132000e-01 /
CHEB / 2.0051000e+00 8.2888000e-01 1.4818000e-01 /
CHEB / -6.1272000e-02 -3.7874000e-02 6.1423000e-02 /
CHEB / -4.6547000e-02 -1.0579000e-01 -3.2507000e-02 /
CHEB / 2.2750000e-02 -2.4414000e-02 -2.4614000e-02 /

CH3CHCHCHO+H(+m)=C3H6+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -7.588678417246198
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1345000e+01 -6.0793000e-01 -1.8865000e-01 /
CHEB / 1.8442000e+00 6.8240000e-01 1.7821000e-01 /
CHEB / -2.3383000e-02 3.1921000e-02 5.0433000e-02 /
CHEB / -6.3878000e-02 -8.6366000e-02 -1.8325000e-02 /
CHEB / -1.5966000e-02 -3.4715000e-02 -2.2306000e-02 /
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CH3CHCHCHO+H(+m)=C3H7-2+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -24.33696963321935
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1017000e+01 -5.5404000e-04 -3.8920000e-04 /
CHEB / 2.0934000e+01 3.7066000e-04 2.5861000e-04 /
CHEB / 1.8314000e-01 2.3613000e-04 1.6743000e-04 /
CHEB / 7.6370000e-02 2.8645000e-05 2.1583000e-05 /
CHEB / 3.3162000e-02 -4.0239000e-05 -2.8543000e-05 /

C3H6+HCO(+m)=C4H7OJ(16)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -16.74845800099176
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2649000e+00 7.0741000e-01 -3.0647000e-01 /
CHEB / 4.3142000e+00 1.7237000e+00 4.7049000e-02 /
CHEB / -1.8335000e+00 3.9194000e-01 1.4633000e-01 /
CHEB / -1.2868000e+00 1.0982000e-02 3.1518000e-02 /
CHEB / -6.8615000e-01 -1.5070000e-01 -3.9167000e-03 /

C3H6+HCO(+m)=C4H7OJ(8)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -28.847231975063288
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1390000e+01 6.4985000e+00 6.5762000e-01 /
CHEB / 3.6877000e+00 -3.5179000e-01 2.5842000e-02 /
CHEB / -1.4741000e+00 -6.2122000e-01 6.7453000e-02 /
CHEB / -8.5544000e-01 -3.1906000e-01 5.4033000e-02 /
CHEB / -4.4213000e-01 -6.2951000e-02 5.3775000e-02 /

C3H6+HCO(+m)=C4H7OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -22.657619962681423
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1666000e+00 1.6423000e+00 -6.9696000e-01 /
CHEB / -3.1128000e-01 2.7213000e+00 1.8564000e-01 /
CHEB / -2.8038000e+00 4.5971000e-01 2.7208000e-01 /
CHEB / -1.4886000e+00 -2.3811000e-01 1.0366000e-01 /
CHEB / -6.1140000e-01 -2.3060000e-01 -1.9649000e-03 /

C3H6+HCO(+m)=C4H7OJ(13)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/Nd     CO_pri_rad
      deltaHrxn(T=298K) = -18.928018237359197 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3109000e+00 8.8281000e-01 -1.0927000e-01 /
CHEB / -8.8687000e-01 9.6345000e-01 4.5553000e-02 /
CHEB / -1.9724000e+00 2.9785000e-01 6.7463000e-02 /
CHEB / -1.0890000e+00 -4.0639000e-02 2.4734000e-02 /
CHEB / -5.2844000e-01 -1.0449000e-01 -1.1586000e-02 /
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C3H6+HCO(+m)=C3H7-2+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -16.748291215973154
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4951000e+01 -1.7162000e-05 -1.3310000e-05 /
CHEB / 2.2916000e+01 5.9450000e-06 3.3382000e-06 /
CHEB / 1.0418000e-01 2.7991000e-05 2.1227000e-05 /
CHEB / 2.4385000e-02 1.4905000e-05 1.2037000e-05 /
CHEB / -2.6192000e-03 -7.9568000e-06 -5.5901000e-06 /

C3H7-2+CO(+m)=C4H7OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -12.098940759090134
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2448000e+01 1.3640000e+01 1.8709000e+00 /
CHEB / 2.7048000e+01 1.0960000e-01 7.4553000e-02 /
CHEB / -1.9698000e+00 -8.6623000e-01 1.5766000e-01 /
CHEB / -1.1885000e+00 -6.5298000e-01 5.6498000e-02 /
CHEB / -5.9360000e-01 -3.2326000e-01 4.3813000e-02 /

C3H7-2+CO(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -5.909328746708271
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0929000e+01 1.3009000e+01 -1.4798000e+00 /
CHEB / 2.4635000e+01 1.5604000e-01 1.1774000e+00 /
CHEB / -3.1386000e+00 -6.3379000e-01 7.8946000e-01 /
CHEB / -1.7752000e+00 -5.9589000e-01 2.5872000e-01 /
CHEB / -8.7372000e-01 -2.6951000e-01 -1.8594000e-02 /

C3H7-2+CO(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -0.800047291313561
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4678000e+01 -3.2152000e-03 -2.3450000e-03 /
CHEB / 3.0192000e+01 1.9697000e-03 1.3985000e-03 /
CHEB / 5.7439000e-01 2.1272000e-03 1.6024000e-03 /
CHEB / 1.8042000e-01 -1.1855000e-04 -6.5634000e-05 /
CHEB / 4.8123000e-02 -7.8606000e-04 -6.0536000e-04 /

C4H7-11+O(+m)=C4H7OJ(16)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -119.04792999415109
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3981000e+01 1.8407000e+01 9.0219000e-01 /
CHEB / -3.9388000e+00 -2.9523000e+00 2.5323000e-01 /
CHEB / -2.6789000e+00 -2.0019000e+00 2.3740000e-01 /
CHEB / -1.4321000e+00 -1.0086000e+00 1.6786000e-01 /
CHEB / -8.0118000e-01 -3.4447000e-01 1.4586000e-01 /
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```
C4H7-11+O(+m)=C4H7OJ(8)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -131.14670396822262
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8302000e+01 1.7782000e+01 4.5539000e+00 /
CHEB / -2.9768000e+00 -1.2542000e+00 -6.4723000e-01 /
CHEB / -2.6472000e+00 -1.5063000e+00 -2.5033000e-01 /
CHEB / -1.3908000e+00 -8.2234000e-01 -9.3958000e-02 /
CHEB / -6.6010000e-01 -3.3967000e-01 4.7392000e-02 /

C4H7-11+O(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Cd_pri_rad     Oa        deltaHrxn(T=298K) = -
124.95709195584075 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8289000e+01 1.9270000e+01 1.0704000e+00 /
CHEB / -4.8653000e+00 -1.8418000e+00 1.9301000e-01 /
CHEB / -3.4466000e+00 -1.7471000e+00 2.7891000e-01 /
CHEB / -1.8230000e+00 -9.7856000e-01 1.1619000e-01 /
CHEB / -9.0472000e-01 -3.6796000e-01 9.1918000e-02 /

C4H7-11+O(+m)=C4H7OJ(13)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -121.22749023051853
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7597000e+01 1.8556000e+01 2.0424000e+00 /
CHEB / -3.1609000e+00 -2.0096000e+00 -3.2117000e-01 /
CHEB / -2.4587000e+00 -1.7266000e+00 -7.5837000e-02 /
CHEB / -1.2978000e+00 -9.2243000e-01 -2.9158000e-02 /
CHEB / -6.5185000e-01 -4.0790000e-01 6.0571000e-02 /

C4H7-11+O(+m)=C2H4+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -100.31952192060608
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0071000e+01 6.7832000e-04 4.6676000e-04 /
CHEB / 3.7942000e-01 -3.0303000e-04 -1.9720000e-04 /
CHEB / -4.2230000e-02 -5.3551000e-04 -3.8354000e-04 /
CHEB / -2.9968000e-02 -1.6267000e-05 -1.2234000e-05 /
CHEB / -1.3252000e-02 1.4760000e-04 1.0689000e-04 /

C4H7-11+O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -119.84781050044604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3783000e+00 -1.9355000e-04 -1.3862000e-04 /
CHEB / 1.1099000e+00 1.3312000e-04 9.6564000e-05 /
CHEB / 3.3730000e-01 9.7323000e-05 6.9172000e-05 /
CHEB / 1.3239000e-01 -2.7795000e-05 -2.0787000e-05 /
CHEB / 5.3661000e-02 -2.7016000e-05 -1.9255000e-05 /
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C4H7-11+O(+m)=C2H5+CH2CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -99.96982753014498
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0468000e+00 -1.0012000e-03 -7.0099000e-04 /
CHEB / 1.4323000e+00 5.1415000e-04 3.6087000e-04 /
CHEB / 4.8179000e-01 6.4443000e-04 4.5138000e-04 /
CHEB / 1.8433000e-01 2.0487000e-05 1.3312000e-05 /
CHEB / 6.4888000e-02 -1.5865000e-04 -1.1156000e-04 /

C4H7-11+O(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -97.5703302676432
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3120000e+01 -1.1976000e-07 -8.3299000e-08 /
CHEB / -1.3651000e-01 3.2047000e-07 2.2365000e-07 /
CHEB / -1.6834000e-02 2.9613000e-08 2.0349000e-08 /
CHEB / 6.2583000e-03 -1.5344000e-07 -1.0750000e-07 /
CHEB / 3.4560000e-03 -1.3340000e-07 -9.2961000e-08 /

C4H7-11+O(+m)=CH3CHCHCHO+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -94.71079357591313
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1274000e+01 -1.6935000e-07 -1.2793000e-07 /
CHEB / 4.8095000e-01 -2.3515000e-06 -1.6380000e-06 /
CHEB / 1.5463000e-01 8.2113000e-07 5.8356000e-07 /
CHEB / 7.1445000e-02 1.6121000e-06 1.1271000e-06 /
CHEB / 3.1391000e-02 8.3966000e-07 5.8148000e-07 /

C4H7-11+O(+m)=C3H6+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -102.29947199315933
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0504000e+01 -3.8952000e-04 -2.7854000e-04 /
CHEB / 7.2821000e-01 2.7347000e-04 1.9695000e-04 /
CHEB / 1.7765000e-01 2.8004000e-04 1.9890000e-04 /
CHEB / 1.9656000e-02 -7.0374000e-05 -5.1775000e-05 /
CHEB / -1.5621000e-02 -1.0430000e-04 -7.3997000e-05 /

C4H7-11+O(+m)=C3H7-2+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7OJ(16))   deltaHrxn(T=298K) = -119.04776320913248
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7187000e+00 -6.0001000e-03 -4.0980000e-03 /
CHEB / 2.7938000e+00 3.2014000e-03 2.1531000e-03 /
CHEB / 1.0271000e+00 4.1137000e-03 2.8288000e-03 /
CHEB / 3.4133000e-01 3.1052000e-05 5.1773000e-05 /
CHEB / 9.4164000e-02 -1.2163000e-03 -8.3535000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown(1)        20.45 77.09 20.03 26.34 32.2  36.68 43.8  48.8
      58.45 null
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+aC3H5=unknown(1)         6.9200000e+10      0.00000
4.3720000e+04
!     CH2CHO+C2H4=unknown(1)        6.9200000e+10      0.00000
4.3720000e+04

CH2CHO+C2H4(+m)=CH2O+aC3H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown)      deltaHrxn(T=298K) = -2.4798291596540736
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9545000e+00 -7.7523000e-01 -1.9287000e-01 /
CHEB / 1.6157000e+01 8.4582000e-01 1.4678000e-01 /
CHEB / 2.5222000e-02 6.4141000e-02 9.5287000e-02 /
CHEB / -1.2986000e-01 -9.6124000e-02 -1.3054000e-02 /
CHEB / -5.7744000e-02 -5.3306000e-02 -3.3540000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     cH2C[O]C2H5       -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     CH3C[O]CH2cH2     -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CH2C[OH]cHCH3     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CH2C[OH]CH2cH2    5.43  85.83 23.53 28.76 33.18 36.91 43.01 47.46
      54.07 null
!     cHC[OH]C2H5       15.53 83.81 24.11 29.37 33.73 37.39 43.35 47.71
      54.2  null
!     CH3C[OH]cCH3      10.22 83.01 24.09 28.56 32.53 36.09 42.21 46.76
      53.62 null
!     cH2CH[OH]C2H3     9.75  85.19 23.45 29.19 34.08 37.79 43.84 48.16
      54.19 null
!     CH3CH[OH]CHcH     19.85 83.17 24.03 29.8  34.63 38.27 44.18 48.41
      54.32 null
```

```
!     CH3CH[OH]cCH2     17.65 83.59 23.88 29.34 34.05 37.67 43.66 47.99
      54.09 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     CH2CO             -10.78      57.63 12.31 14.11 15.57 16.77 18.67
      20.12 22.44
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C4H6O(717)        -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92
      50.63 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C3H4O-enone       -13.82      68.58 16.45 19.54 22.36 24.81 28.75
      31.71 36.31
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H3O-2           28.54 64.12 14.36 16.86 18.74 20.19 22.32 23.9
      26.53
!     HCCOH       23.15 59.1  13.44 15.17 16.46 17.47 19.01 20.21 22.29
!     C4H6-1            42.02 69.18 19.47 23.9  27.69 30.86 35.89 39.71
      45.81
!     C4H6-2            34.7  67.78 18.64 22.64 26.42 29.76 35.24 39.38
      47.86 null
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C2H2              56.1  47.73 10.27 11.79 12.85 13.67 14.94 15.97
      17.79
!     nC4H5       85.18 69.37 18.93 23.55 27.16 29.92 34.02 37.03 41.81
      null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H3OH            4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94
      36.79 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
```

```
!     C4H7-12           56.79 75.42 20.23 24.88 29.1  32.76 38.62 43.06
      49.99 null
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+C2H5=cH2C[O]C2H5  1.9263655e+11      0.04067
9.2900000e+03
!     cH2C[O]C2H5=CH3C[O]CH2cH2     2.2860000e+10      0.35000
1.9760000e+04
!     CH3CO+C2H4=CH3C[O]CH2cH2      5.2000000e+11      0.00000
6.5600000e+03
!     C4H6O(717)+H=CH3C[O]CH2cH2    2.8500000e+13      0.00000
4.3000000e+03
!     C3H7-1+CO=CH3C[O]CH2cH2 5.3800000e+02      3.29000
1.0450000e+05
!     CH3C[O]CH2cH2=CH3C[O]cHCH3    5.6400000e+08      1.28000
2.7900000e+04
!     CH3+C3H4O-enone=CH3C[O]cHCH3  2.8149495e+12      0.00000
7.8566667e+03
!     C4H6O(717)+H=CH3C[O]cHCH3     3.7100000e+13      0.00000
1.0000000e+03
!     cH2C[O]C2H5=CH3C[O]cHCH3      2.3600000e+10      0.82000
3.5100000e+04
!     CH3C[O]cHCH3=CH3C[OH]CHcH2    3.5266395e+10      0.61833
2.7168333e+04
!     C4H6O(717)+H=CH3C[OH]CHcH2    2.3501400e+11      0.30815
4.9629937e+03
!     CH2C[OH]cHCH3=CH3C[OH]CHcH2   1.8288499e+09      1.13906
3.4790987e+04
!     C4H6-12+OH=CH2C[OH]cHCH3      2.7411173e+10      0.56667
3.7888889e+03
!     CH2C[OH]CH2cH2=CH2C[OH]cHCH3  5.6400000e+08      1.28000
2.7900000e+04
!     C2H3O-2+C2H4=CH2C[OH]CH2cH2   7.2400000e+12      0.00000
4.5000000e+03
!     cHC[OH]C2H5=CH2C[OH]CH2cH2    1.8288499e+09      1.13906
3.4790987e+04
!     HCCOH+C2H5=cHC[OH]C2H5  1.9988684e+10      0.00000
6.9750000e+03
!     C4H6-1+OH=cHC[OH]C2H5   7.6000000e+07      1.70000
1.0000000e+03
!     cHC[OH]C2H5=CH2C[OH]cHCH3     3.6920000e+10      0.74000
3.4700000e+04
!     cH2C[O]C2H5=cHC[OH]C2H5       8.1282219e+08      1.13906
3.4790987e+04
!     cH2C[O]C2H5=CH2C[OH]CH2cH2    9.0000000e+11      0.00000
2.9400000e+04
!     CH2C[OH]CH2cH2=C4H7OJ(272)    1.0000000e+10      0.00000
2.5850000e+04
!     CH2C[OH]CH2cH2=C4H7OJ(273)    7.9257121e+07      1.09000
3.4816450e+04
!     cH2C[O]C2H5=CH2C[OH]cHCH3     9.7200000e+09      1.17000
3.9660000e+04
!     CH3C[OH]cCH3=CH2C[OH]cHCH3    2.3220000e+10      1.08000
3.8700000e+04
!     C4H6-2+OH=CH3C[OH]cCH3  7.6000000e+07      1.70000
1.0000000e+03
!     CH3C[OH]cCH3=CH3C[OH]CHcH2    2.1960000e+10      1.12000
4.1300000e+04
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!     CH3C[O]cHCH3=CH3C[OH]cCH3     2.0320555e+08      1.13906
3.4790987e+04
!     CH3C[O]cHCH3=CH2C[OH]cHCH3    4.2390000e+09      1.45000
4.2270000e+04
!     cH2CH[OH]C2H3=CH3C[OH]CHcH2   6.2339791e+09      0.93630
3.7689907e+04
!     C2H4O+C2H3=cH2CH[OH]C2H3      1.4902950e+02      3.00740
1.0170800e+04
!     C4H6-13+OH=cH2CH[OH]C2H3      2.7100000e+12      0.00000
0.0000000e+00
!     CH3CH[OH]CHcH=cH2CH[OH]C2H3   1.8288499e+09      1.13906
3.4790987e+04
!     C2H5O-2+C2H2=CH3CH[OH]CHcH    2.5050000e+10      0.00000
6.9000000e+03
!     nC4H5+H2O=CH3CH[OH]CHcH 6.5200000e+01      2.92000
5.0700000e+04
!     CH3CH[OH]CHcH=CH3CH[OH]cCH2   3.2400000e+11      0.73000
4.2400000e+04
!     CH3+C3H3OH=CH3CH[OH]cCH2      8.8574827e+11      0.00000
1.0000000e+04
!     C4H6-12+OH=CH3CH[OH]cCH2      2.7411173e+10      0.56667
3.7888889e+03
!     CH3CH[OH]cCH2=CH3C[OH]CHcH2   6.6570470e+09      0.91000
3.8200000e+04
!     CH3CH[OH]cCH2=cH2CH[OH]C2H3   6.9120000e+09      1.24000
3.6300000e+04
!     CH3CH[o]C2H3=CH3CH[OH]cCH2    2.0320555e+08      1.13906
3.4790987e+04
!     CH3+C3H4O=CH3CH[o]C2H3  3.1600000e+10      0.00000
1.1510000e+04
!     CH3CHO+C2H3=CH3CH[o]C2H3      3.2847733e+07      1.50370
7.3354000e+03
!     C4H6O(717)+H=CH3CH[o]C2H3     1.0000000e+11      0.00000
1.1900000e+04
!     CH3CH[o]C2H3=CH3C[OH]CHcH2    2.0320555e+08      1.13906
3.4790987e+04
!     CH3CH[o]C2H3=CH3CH[OH]CHcH    8.1282219e+08      1.13906
3.4790987e+04
!     CH3CH[o]C2H3=cH2CH[OH]C2H3    4.2390000e+09      1.45000
4.2270000e+04
!     C4H7-24+O=CH3CH[o]C2H3  1.0000000e+13      0.00000
0.0000000e+00
!     CH3CH[OH]CHcH=CH3C[OH]CHcH2   6.4169055e+09      0.87916
3.6978100e+04
!     C4H7-22+O=CH3C[O]cHCH3  1.0000000e+13      0.00000
0.0000000e+00
!     C4H7-12+O=cH2C[O]C2H5   1.0000000e+13      0.00000
0.0000000e+00
!     cH2C[O]C2H5=C4H7OJ(88)        7.9257121e+07      1.09000
3.4816450e+04

cH2C[O]C2H5(+m)=CH3C[O]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.8996711952396472 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -3.2267000e+00 9.6867000e-02 -2.6475000e-01 /
CHEB / 6.1488000e+00 1.8561000e+00 1.0425000e-01 /
CHEB / -3.1692000e+00 2.9225000e-01 1.0108000e-01 /
CHEB / -1.9776000e+00 -2.8308000e-01 2.9998000e-02 /
CHEB / -9.3247000e-01 -3.0588000e-01 -3.3673000e-02 /

cH2C[O]C2H5(+m)=CH3C[OH]CHcH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.699741612302213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9524000e+00 -7.5111000e-01 -2.8525000e-01 /
CHEB / 7.8400000e+00 2.6654000e+00 1.5221000e-01 /
CHEB / -3.0473000e+00 3.7722000e-01 1.7468000e-01 /
CHEB / -2.0384000e+00 -3.0058000e-01 6.4695000e-02 /
CHEB / -9.9328000e-01 -3.6155000e-01 -4.4012000e-02 /

cH2C[O]C2H5(+m)=CH2C[OH]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) R3H_SS_2Cd     O_rad_out     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.699741612302213 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0699000e+00 1.5669000e+00 -1.3258000e-01 /
CHEB / 9.0504000e+00 1.3563000e+00 6.4640000e-02 /
CHEB / -3.0009000e+00 1.6515000e-01 1.6527000e-01 /
CHEB / -1.8260000e+00 -1.9277000e-01 2.1259000e-02 /
CHEB / -9.0658000e-01 -2.8101000e-01 -3.6401000e-02 /

CH3C[O]CH2cH2(+m)=cH2C[O]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7094000e-01 6.5131000e-01 -5.3363000e-02 /
CHEB / 2.4000000e+00 9.2120000e-01 -2.5702000e-02 /
CHEB / -3.1099000e+00 2.3790000e-01 5.5337000e-02 /
CHEB / -1.8116000e+00 -2.0009000e-01 3.8740000e-02 /
CHEB / -8.2278000e-01 -2.7535000e-01 -1.9645000e-02 /

CH3C[O]CH2cH2(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -2.8996711952396472 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2245000e+00 1.1703000e+00 -1.8106000e-01 /
CHEB / 5.2198000e+00 9.6363000e-01 9.6453000e-02 /
CHEB / -3.1749000e+00 2.0994000e-01 6.1893000e-02 /
CHEB / -1.8572000e+00 -1.6875000e-01 1.0502000e-02 /
CHEB / -8.6485000e-01 -2.1687000e-01 -2.5913000e-02 /

CH3C[O]CH2cH2(+m)=CH3C[OH]CHcH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.699741612302213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1801000e+00 8.1750000e-02 -2.3647000e-01 /
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CHEB / 6.9838000e+00 1.8085000e+00 1.4179000e-01 /
CHEB / -2.9945000e+00 3.5190000e-01 1.2675000e-01 /
CHEB / -1.9687000e+00 -2.3582000e-01 3.4833000e-02 /
CHEB / -9.6202000e-01 -3.1081000e-01 -3.1772000e-02 /

CH3C[O]CH2cH2(+m)=CH2C[OH]cHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.699741612302213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8110000e+00 6.9299000e-01 -2.1143000e-01 /
CHEB / 9.6481000e+00 1.9936000e+00 3.7871000e-02 /
CHEB / -2.8999000e+00 2.8723000e-01 1.7889000e-01 /
CHEB / -1.8560000e+00 -1.9721000e-01 4.0267000e-02 /
CHEB / -9.2980000e-01 -3.1212000e-01 -3.4093000e-02 /

CH3C[OH]CHcH2(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.19992958293743435
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4762000e-01 6.4921000e-01 -4.2386000e-02 /
CHEB / 4.9586000e+00 9.5810000e-01 -1.3803000e-02 /
CHEB / -3.0401000e+00 3.1778000e-01 6.4581000e-02 /
CHEB / -1.8239000e+00 -1.2852000e-01 5.1093000e-02 /
CHEB / -8.9051000e-01 -2.5087000e-01 -8.1307000e-03 /

CH2C[OH]cHCH3(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.19992958293743435
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1049000e+00 -2.5955000e-03 -1.4122000e-01 /
CHEB / 8.7988000e+00 2.2421000e+00 1.2726000e-02 /
CHEB / -2.9897000e+00 4.5628000e-01 7.7414000e-02 /
CHEB / -1.8652000e+00 -1.8815000e-01 5.9813000e-02 /
CHEB / -9.0165000e-01 -2.6179000e-01 -4.4971000e-04 /

CH2C[OH]cHCH3(+m)=CH3C[OH]CHcH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) R4H_SDS     C_rad_out_2H     Cs_H_out_2H
      deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9980000e+00 9.8915000e-01 -1.7090000e-01 /
CHEB / 8.4012000e+00 1.1969000e+00 -4.6327000e-02 /
CHEB / -2.5934000e+00 4.0544000e-01 6.0778000e-02 /
CHEB / -1.6327000e+00 -7.9488000e-02 4.8686000e-02 /
CHEB / -8.6768000e-01 -2.4352000e-01 -2.8960000e-03 /

CH2C[OH]CH2cH2(+m)=cH2C[O]C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.308686028694982
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7919000e+00 1.2399000e+00 -2.0905000e-01 /
CHEB / -1.1077000e-01 1.2137000e+00 5.5382000e-02 /
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CHEB / -3.5805000e+00 8.0436000e-02 1.4373000e-01 /
CHEB / -1.9086000e+00 -3.8368000e-01 2.5166000e-02 /
CHEB / -7.8059000e-01 -3.4182000e-01 -6.5644000e-02 /

CH2C[OH]CH2cH2(+m)=CH3C[O]CH2cH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
13.308686028694982 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1196000e-01 1.9814000e-01 -3.3415000e-01 /
CHEB / 7.7765000e-01 1.9344000e+00 1.0563000e-01 /
CHEB / -3.5047000e+00 2.1923000e-01 1.7251000e-01 /
CHEB / -1.9729000e+00 -4.3071000e-01 2.4579000e-02 /
CHEB / -8.2488000e-01 -3.9336000e-01 -7.4260000e-02 /

CH2C[OH]CH2cH2(+m)=CH3C[O]cHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.20835722393463
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4150000e+00 -3.8049000e-01 -3.1047000e-01 /
CHEB / 2.7374000e+00 2.5830000e+00 1.2316000e-01 /
CHEB / -3.4238000e+00 1.8564000e-01 1.6213000e-01 /
CHEB / -2.0208000e+00 -4.5289000e-01 1.8625000e-02 /
CHEB / -8.5402000e-01 -3.9771000e-01 -8.1298000e-02 /

CH2C[OH]CH2cH2(+m)=CH3C[OH]CHcH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
16.008427640997198 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6991000e+00 -1.0501000e+00 -3.3200000e-01 /
CHEB / 4.1523000e+00 3.2941000e+00 2.2168000e-01 /
CHEB / -3.3020000e+00 2.5695000e-01 2.4086000e-01 /
CHEB / -2.0385000e+00 -4.9298000e-01 1.3158000e-02 /
CHEB / -8.8533000e-01 -4.3343000e-01 -8.9366000e-02 /

CH2C[OH]CH2cH2(+m)=CH2C[OH]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -16.008427640997198 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7589000e+00 1.7045000e+00 -2.2981000e-01 /
CHEB / 4.4499000e+00 1.5865000e+00 1.3705000e-01 /
CHEB / -3.2433000e+00 -7.3969000e-03 2.1233000e-01 /
CHEB / -1.7957000e+00 -3.7082000e-01 1.2922000e-02 /
CHEB / -7.8171000e-01 -3.3865000e-01 -6.6326000e-02 /

CH2C[OH]CH2cH2(+m)=C3H7-1+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.659454822271368
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2409000e+01 1.7007000e+01 1.1553000e-01 /
CHEB / 2.9622000e+01 -1.7545000e+00 1.5592000e+00 /
CHEB / -2.2243000e+00 -1.6401000e+00 -1.1861000e-01 /
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CHEB / -1.2286000e+00 -8.6338000e-01 -9.4268000e-02 /
CHEB / -6.3079000e-01 -2.6479000e-01 4.6050000e-02 /

cHC[OH]C2H5(+m)=cH2C[O]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.407587312915595
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7682000e+00 2.0752000e+00 -5.5250000e-01 /
CHEB / -1.2176000e+00 1.2220000e+00 1.3261000e-01 /
CHEB / -3.0051000e+00 -1.1012000e-01 1.6664000e-01 /
CHEB / -1.5205000e+00 -3.2359000e-01 1.9519000e-03 /
CHEB / -6.5022000e-01 -1.9393000e-01 -4.3335000e-02 /

cHC[OH]C2H5(+m)=CH3C[O]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.407587312915595
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8139000e+00 1.1813000e+00 -6.7443000e-01 /
CHEB / -4.9373000e-01 1.7249000e+00 1.5548000e-01 /
CHEB / -2.9380000e+00 7.6006000e-03 1.7236000e-01 /
CHEB / -1.5658000e+00 -3.4818000e-01 -1.3079000e-03 /
CHEB / -6.8937000e-01 -2.3820000e-01 -4.8727000e-02 /

cHC[OH]C2H5(+m)=CH3C[O]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -26.307258508155243
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2557000e+00 4.1539000e-01 -4.8652000e-01 /
CHEB / 8.6712000e-01 2.2547000e+00 1.0287000e-01 /
CHEB / -2.8340000e+00 1.5270000e-01 7.6638000e-02 /
CHEB / -1.5810000e+00 -2.9986000e-01 -3.4174000e-02 /
CHEB / -7.1436000e-01 -2.3356000e-01 -4.1417000e-02 /

cHC[OH]C2H5(+m)=CH3C[OH]CHcH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -26.107328925217807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2819000e-01 -4.3683000e-01 -5.1480000e-01 /
CHEB / 2.0575000e+00 2.8662000e+00 2.4644000e-01 /
CHEB / -2.6412000e+00 1.8595000e-01 1.4009000e-01 /
CHEB / -1.5697000e+00 -3.3295000e-01 -2.6174000e-02 /
CHEB / -7.4897000e-01 -2.7359000e-01 -4.3549000e-02 /

cHC[OH]C2H5(+m)=CH2C[OH]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
R3H_DS     Cd_rad_out_singleH     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -26.107328925217807 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4479000e-02 1.2901000e+00 -3.9072000e-01 /
CHEB / 2.4229000e+00 1.8037000e+00 4.2060000e-01 /
CHEB / -2.3692000e+00 -4.5366000e-02 1.1888000e-01 /
CHEB / -1.3568000e+00 -2.8435000e-01 -6.3335000e-02 /
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CHEB / -6.7141000e-01 -2.0019000e-01 -4.9536000e-02 /

cHC[OH]C2H5(+m)=CH2C[OH]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) R4H_DSS     Cd_rad_out_singleH     Cs_H_out_2H
      deltaHrxn(T=298K) = -10.098901284220611 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1686000e+00 1.0269000e+00 -5.6243000e-01 /
CHEB / -7.8915000e-01 2.0807000e+00 2.0680000e-01 /
CHEB / -3.1501000e+00 -9.2081000e-02 1.5800000e-01 /
CHEB / -1.5530000e+00 -4.9717000e-01 -5.7652000e-02 /
CHEB / -5.7626000e-01 -2.9529000e-01 -8.6349000e-02 /

cHC[OH]C2H5(+m)=CH3C[OH]cCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.309515492096409
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6835000e+00 -1.3746000e-01 -4.6676000e-01 /
CHEB / 2.8306000e+00 2.7837000e+00 2.8648000e-01 /
CHEB / -2.3345000e+00 -4.1508000e-02 1.3078000e-01 /
CHEB / -1.3172000e+00 -4.2356000e-01 -6.5494000e-02 /
CHEB / -5.8667000e-01 -2.5119000e-01 -6.6421000e-02 /

cHC[OH]C2H5(+m)=cH2CH[OH]C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.779293284249826
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1992000e+01 4.4815000e+00 -1.5446000e+00 /
CHEB / 7.3417000e+00 2.7071000e+00 8.0763000e-01 /
CHEB / -2.6294000e+00 -4.5405000e-02 2.4542000e-01 /
CHEB / -1.4740000e+00 -4.1069000e-01 -2.0632000e-03 /
CHEB / -7.2566000e-01 -2.9191000e-01 -6.4361000e-02 /

cHC[OH]C2H5(+m)=CH3CH[o]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.819555404457633
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6863000e+01 6.5000000e+00 -1.8882000e+00 /
CHEB / 6.3406000e+00 1.6313000e+00 9.0655000e-01 /
CHEB / -3.0464000e+00 -4.1920000e-01 2.0741000e-01 /
CHEB / -1.5141000e+00 -4.6584000e-01 -2.3594000e-02 /
CHEB / -6.3268000e-01 -2.3647000e-01 -6.0585000e-02 /

cHC[OH]C2H5(+m)=CH2CO+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 3.119626863809078
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1789000e+00 1.0665000e+00 -4.0586000e-01 /
CHEB / 1.4431000e+00 2.1367000e+00 3.0566000e-01 /
CHEB / -1.9951000e+00 1.1195000e-01 1.6565000e-01 /
CHEB / -9.9577000e-01 -1.9108000e-01 -3.0687000e-02 /
CHEB / -4.4346000e-01 -1.0365000e-01 -4.1862000e-02 /
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cHC[OH]C2H5(+m)=CH3CO+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.9293234229070304
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1198000e+00 -2.1246000e-01 -4.7782000e-01 /
CHEB / 1.2825000e+00 2.1384000e+00 3.5318000e-01 /
CHEB / -1.9427000e+00 2.2917000e-01 1.6180000e-01 /
CHEB / -1.0366000e+00 -1.7566000e-01 -2.1917000e-02 /
CHEB / -4.7876000e-01 -1.1329000e-01 -4.1121000e-02 /

cHC[OH]C2H5(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.75835610649198
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7620000e+01 1.3975000e+01 2.1815000e+00 /
CHEB / 2.6698000e+01 -1.8168000e+00 5.4921000e-01 /
CHEB / -1.6516000e+00 -4.5846000e-01 -1.9316000e-01 /
CHEB / -9.3889000e-01 -3.6554000e-01 -1.4768000e-01 /
CHEB / -5.0498000e-01 -2.0959000e-01 -3.3806000e-02 /

CH3C[OH]cCH3(+m)=cH2C[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.098071820819186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8881000e-01 2.6968000e-02 -4.0752000e-01 /
CHEB / 3.0038000e+00 2.4449000e+00 1.2491000e-01 /
CHEB / -2.8625000e+00 2.5827000e-01 1.6994000e-01 /
CHEB / -1.7935000e+00 -3.8144000e-01 2.3333000e-02 /
CHEB / -8.2264000e-01 -3.5958000e-01 -6.6426000e-02 /

CH3C[OH]cCH3(+m)=CH3C[O]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.098071820819186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6654000e-02 7.1795000e-01 -3.3335000e-01 /
CHEB / 2.4200000e+00 1.7470000e+00 1.3070000e-01 /
CHEB / -2.8249000e+00 2.4833000e-01 1.0079000e-01 /
CHEB / -1.7445000e+00 -3.1854000e-01 1.6299000e-02 /
CHEB / -7.9462000e-01 -3.1304000e-01 -4.5399000e-02 /

CH3C[OH]cCH3(+m)=CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.997743016058834
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4860000e+00 1.0694000e+00 -1.3783000e-01 /
CHEB / 2.1801000e-01 1.3814000e+00 -6.6936000e-02 /
CHEB / -3.0596000e+00 3.1401000e-01 7.5483000e-02 /
CHEB / -1.6836000e+00 -2.1260000e-01 3.4262000e-02 /
CHEB / -7.5385000e-01 -2.5464000e-01 -3.1414000e-02 /
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CH3C[OH]cCH3(+m)=CH3C[OH]CHcH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
Others-R2H_S    Cd_rad_out_double     Cs_H_out_2H
      deltaHrxn(T=298K) = -20.797813433121398 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2015000e+00 -3.1376000e-02 -2.6493000e-01 /
CHEB / 1.6938000e+00 2.1806000e+00 9.7438000e-03 /
CHEB / -2.8356000e+00 3.9351000e-01 1.6623000e-01 /
CHEB / -1.7065000e+00 -3.0887000e-01 3.6160000e-02 /
CHEB / -8.0615000e-01 -3.3529000e-01 -5.8028000e-02 /

CH3C[OH]cCH3(+m)=CH2C[OH]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
R3H_DS     Cd_rad_out_singleNd     Cs_H_out_2H        deltaHrxn(T=298K)
= -20.797813433121398 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1142000e+00 -5.5960000e-01 -1.9038000e-01 /
CHEB / 4.1634000e+00 2.9173000e+00 2.2893000e-02 /
CHEB / -2.5391000e+00 3.1763000e-01 1.6037000e-01 /
CHEB / -1.5802000e+00 -3.0434000e-01 3.1365000e-02 /
CHEB / -7.6365000e-01 -3.0126000e-01 -6.0260000e-02 /

CH3C[OH]cCH3(+m)=CH2C[OH]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.789385792124202
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1517000e+00 -4.7213000e-01 -4.9304000e-01 /
CHEB / 3.4974000e+00 3.1173000e+00 2.3045000e-01 /
CHEB / -3.0436000e+00 1.1109000e-01 2.3148000e-01 /
CHEB / -1.7805000e+00 -5.8315000e-01 -3.4879000e-02 /
CHEB / -7.1591000e-01 -4.2425000e-01 -1.1370000e-01 /

CH3C[OH]cCH3(+m)=cH2CH[OH]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.4697777921534172
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1661000e+01 4.3393000e+00 -1.6161000e+00 /
CHEB / 8.2530000e+00 2.4247000e+00 6.8010000e-01 /
CHEB / -2.9979000e+00 9.0889000e-02 2.5083000e-01 /
CHEB / -1.6639000e+00 -4.1954000e-01 -7.8121000e-04 /
CHEB / -7.7011000e-01 -3.4112000e-01 -8.1356000e-02 /

CH3C[OH]cCH3(+m)=CH3CO+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 1.3801920691893788
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6324000e+00 -6.9323000e-01 -3.1514000e-01 /
CHEB / 4.2834000e+00 2.3999000e+00 1.4716000e-01 /
CHEB / -1.8456000e+00 4.4124000e-01 1.4282000e-01 /
CHEB / -1.1987000e+00 -1.9961000e-01 2.1345000e-02 /
CHEB / -5.6565000e-01 -2.0143000e-01 -4.5234000e-02 /
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CH3C[OH]cCH3(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.44884061439557
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9944000e+01 1.5154000e+01 8.3648000e-01 /
CHEB / 2.9003000e+01 -1.6615000e+00 1.0966000e+00 /
CHEB / -1.4591000e+00 -1.0361000e+00 -3.7833000e-01 /
CHEB / -8.9921000e-01 -4.8910000e-01 -1.4869000e-01 /
CHEB / -5.5896000e-01 -1.9569000e-01 3.4411000e-02 /

cH2CH[OH]C2H3(+m)=cH2C[O]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -17.628294028665767
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1577000e+01 4.6811000e+00 -1.6927000e+00 /
CHEB / 8.5207000e+00 2.6489000e+00 7.0621000e-01 /
CHEB / -3.4098000e+00 2.4884000e-01 3.0055000e-01 /
CHEB / -2.0409000e+00 -3.7001000e-01 2.1066000e-03 /
CHEB / -9.6969000e-01 -3.8735000e-01 -7.2428000e-02 /

cH2CH[OH]C2H3(+m)=CH3C[O]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -17.628294028665767
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1805000e+01 4.7700000e+00 -1.4325000e+00 /
CHEB / 8.6827000e+00 2.3681000e+00 4.0114000e-01 /
CHEB / -3.4232000e+00 2.9294000e-01 2.4973000e-01 /
CHEB / -2.0221000e+00 -3.1090000e-01 4.3417000e-02 /
CHEB / -9.5662000e-01 -3.6315000e-01 -4.2817000e-02 /

cH2CH[OH]C2H3(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.527965223905415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7180000e+00 4.7680000e+00 -1.3144000e+00 /
CHEB / 6.9115000e+00 2.1523000e+00 3.7249000e-01 /
CHEB / -3.7073000e+00 3.3570000e-01 1.9455000e-01 /
CHEB / -2.0015000e+00 -2.8119000e-01 3.9297000e-02 /
CHEB / -9.2696000e-01 -3.3147000e-01 -4.2381000e-02 /

cH2CH[OH]C2H3(+m)=CH3C[OH]CHcH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_2H     Cs_H_out
      deltaHrxn(T=298K) = -20.328035640967983 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3094000e+00 5.3832000e+00 -1.1765000e+00 /
CHEB / 7.4404000e+00 1.7068000e+00 2.3335000e-01 /
CHEB / -3.3997000e+00 3.1269000e-01 1.7069000e-01 /
CHEB / -1.8805000e+00 -2.4866000e-01 5.7926000e-02 /
CHEB / -9.0411000e-01 -3.1854000e-01 -2.8355000e-02 /
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cH2CH[OH]C2H3(+m)=CH2C[OH]cHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.328035640967983
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0412000e+00 2.9864000e+00 -1.1263000e+00 /
CHEB / 8.2639000e+00 3.0006000e+00 1.5671000e-01 /
CHEB / -3.2214000e+00 5.6749000e-01 2.6444000e-01 /
CHEB / -1.8477000e+00 -2.3476000e-01 6.8486000e-02 /
CHEB / -9.0368000e-01 -3.1461000e-01 -4.4179000e-02 /

cH2CH[OH]C2H3(+m)=CH2C[OH]CH2cH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
4.319607999970785 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3221000e+01 4.4788000e+00 -1.8153000e+00 /
CHEB / 8.2642000e+00 3.1899000e+00 8.2802000e-01 /
CHEB / -3.6297000e+00 5.2988000e-02 3.6645000e-01 /
CHEB / -2.0154000e+00 -6.1884000e-01 -1.7423000e-02 /
CHEB / -8.3506000e-01 -4.4545000e-01 -1.2115000e-01 /

cH2CH[OH]C2H3(+m)=CH3CO+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 1.849969861342796
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.1353000e+00 9.8387000e-01 -7.3100000e-01 /
CHEB / 1.0970000e+01 1.9618000e+00 3.8008000e-01 /
CHEB / -2.1020000e+00 4.5055000e-01 1.4929000e-01 /
CHEB / -1.3333000e+00 -9.6353000e-02 2.1490000e-02 /
CHEB / -6.7753000e-01 -1.7287000e-01 -2.6001000e-02 /

cH2CH[OH]C2H3(+m)=C3H7-1+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.979062822242152
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7810000e+01 1.4633000e+01 -6.6523000e-01 /
CHEB / 3.0754000e+01 -1.8621000e+00 1.2325000e+00 /
CHEB / -1.6861000e+00 -1.4193000e+00 4.2803000e-01 /
CHEB / -1.2409000e+00 -5.7445000e-01 8.4396000e-02 /
CHEB / -7.9939000e-01 -8.0263000e-02 -4.0318000e-02 /

CH3CH[OH]CHcH(+m)=cH2C[O]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.727195312494633
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2346000e+01 5.9643000e+00 -1.4310000e+00 /
CHEB / 7.7012000e+00 2.5956000e+00 7.3082000e-01 /
CHEB / -3.2716000e+00 -1.4403000e-01 4.9157000e-01 /
CHEB / -1.9884000e+00 -3.9356000e-01 -9.0178000e-03 /
CHEB / -9.6280000e-01 -3.5598000e-01 -1.0074000e-01 /
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CH3CH[OH]CHcH(+m)=CH3C[O]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.727195312494633
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2768000e+01 5.8344000e+00 -1.1536000e+00 /
CHEB / 8.0228000e+00 2.4814000e+00 3.9010000e-01 /
CHEB / -3.2424000e+00 -5.2087000e-02 4.3536000e-01 /
CHEB / -1.9746000e+00 -3.2718000e-01 5.1174000e-02 /
CHEB / -9.6063000e-01 -3.4268000e-01 -6.6431000e-02 /

CH3CH[OH]CHcH(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.62686650773428
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0831000e+01 5.8158000e+00 -8.5000000e-01 /
CHEB / 6.3404000e+00 2.2118000e+00 2.1191000e-01 /
CHEB / -3.4816000e+00 8.0145000e-03 2.8856000e-01 /
CHEB / -1.9664000e+00 -2.7364000e-01 8.4752000e-02 /
CHEB / -9.2791000e-01 -3.0233000e-01 -5.0844000e-02 /

CH3CH[OH]CHcH(+m)=CH3C[OH]CHcH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) R3H_DS     Cd_rad_out_singleH     Cs_H_out
      deltaHrxn(T=298K) = -30.42693692479685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0480000e+01 6.3232000e+00 -7.6710000e-01 /
CHEB / 6.9090000e+00 1.8591000e+00 1.3357000e-01 /
CHEB / -3.1919000e+00 -3.2490000e-02 2.6820000e-01 /
CHEB / -1.8640000e+00 -2.7023000e-01 9.3470000e-02 /
CHEB / -9.1332000e-01 -2.9971000e-01 -4.1049000e-02 /

CH3CH[OH]CHcH(+m)=CH2C[OH]cHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.42693692479685
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7735000e+00 4.2035000e+00 -1.0269000e+00 /
CHEB / 7.4029000e+00 2.9812000e+00 3.4153000e-01 /
CHEB / -3.1082000e+00 1.6395000e-01 4.3829000e-01 /
CHEB / -1.8061000e+00 -2.4477000e-01 5.1590000e-02 /
CHEB / -9.0315000e-01 -2.6852000e-01 -6.4518000e-02 /

CH3CH[OH]CHcH(+m)=CH2C[OH]CH2cH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
14.41850928379965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3813000e+01 5.9593000e+00 -1.5547000e+00 /
CHEB / 7.3044000e+00 2.9473000e+00 8.5651000e-01 /
CHEB / -3.5114000e+00 -3.7142000e-01 5.5004000e-01 /
CHEB / -1.9553000e+00 -6.3096000e-01 -1.4845000e-02 /
CHEB / -8.2063000e-01 -4.0691000e-01 -1.3661000e-01 /
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CH3CH[OH]CHcH(+m)=cHC[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.3196079995790395
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5344000e+01 5.8587000e+00 -1.2068000e+00 /
CHEB / 8.3939000e+00 2.4257000e+00 8.0133000e-01 /
CHEB / -2.4740000e+00 -4.2122000e-01 4.5460000e-01 /
CHEB / -1.4178000e+00 -4.1594000e-01 1.8712000e-03 /
CHEB / -7.1768000e-01 -2.6749000e-01 -9.1039000e-02 /

CH3CH[OH]CHcH(+m)=CH3C[OH]cCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.629123491675449
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3327000e+01 5.6721000e+00 -1.1632000e+00 /
CHEB / 7.5870000e+00 2.2595000e+00 5.3854000e-01 /
CHEB / -2.8277000e+00 -2.9881000e-01 3.2507000e-01 /
CHEB / -1.6302000e+00 -4.0871000e-01 2.9789000e-02 /
CHEB / -7.6713000e-01 -3.0601000e-01 -8.4135000e-02 /

CH3CH[OH]CHcH(+m)=cH2CH[OH]C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) R4H_DSS     Cd_rad_out_singleH     Cs_H_out_2H
      deltaHrxn(T=298K) = -10.098901283828866 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8401000e+00 3.0415000e+00 -8.2372000e-01 /
CHEB / 7.3547000e+00 1.4677000e+00 2.2783000e-01 /
CHEB / -3.0002000e+00 2.7664000e-01 1.7311000e-01 /
CHEB / -1.7464000e+00 -2.1064000e-01 4.3632000e-02 /
CHEB / -8.8172000e-01 -2.8195000e-01 -3.6885000e-02 /

CH3CH[OH]CHcH(+m)=CH3CH[OH]cCH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
R2H_D     Cd_rad_out_singleH     Cd_H_out_singleNd
      deltaHrxn(T=298K) = -2.1997754799544325 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4361000e+00 1.9623000e+00 -1.2449000e-01 /
CHEB / 8.5323000e+00 2.3936000e+00 1.9895000e-02 /
CHEB / -2.5564000e+00 -4.6031000e-02 8.8369000e-04 /
CHEB / -1.6802000e+00 -3.4845000e-01 8.5682000e-02 /
CHEB / -7.7119000e-01 -2.1795000e-01 -1.6866000e-02 /

CH3CH[OH]CHcH(+m)=CH3CH[o]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.1391634040366725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6555000e+00 3.6339000e+00 -6.0204000e-01 /
CHEB / 4.2356000e+00 2.4692000e-01 3.0433000e-01 /
CHEB / -3.2722000e+00 -1.7101000e-01 7.6367000e-02 /
CHEB / -1.6987000e+00 -2.6715000e-01 -2.0965000e-02 /
CHEB / -7.2539000e-01 -1.8079000e-01 -4.0404000e-02 /
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CH3CH[OH]CHcH(+m)=CH2CO+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.1999811357699635
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0163000e+00 3.0970000e-01 -5.5675000e-01 /
CHEB / 1.1196000e+01 1.9864000e+00 3.4333000e-01 /
CHEB / -1.9103000e+00 4.7350000e-01 1.3291000e-01 /
CHEB / -1.3105000e+00 -8.0470000e-02 7.9277000e-03 /
CHEB / -6.9490000e-01 -1.6222000e-01 -2.1684000e-02 /

CH3CH[OH]CHcH(+m)=CH3CO+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -8.248931422486072
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5094000e+00 6.9801000e-01 -3.4771000e-01 /
CHEB / 1.1159000e+01 1.3243000e+00 1.4819000e-01 /
CHEB / -1.8879000e+00 4.1093000e-01 7.4373000e-02 /
CHEB / -1.2763000e+00 -9.8927000e-04 2.7309000e-02 /
CHEB / -6.9001000e-01 -1.2650000e-01 -2.9746000e-03 /

CH3CH[OH]CHcH(+m)=C3H7-1+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.07796410607102
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0998000e+01 1.1430000e+01 -7.3812000e-01 /
CHEB / 2.8117000e+01 -1.3346000e+00 9.9235000e-01 /
CHEB / -1.8697000e+00 -8.7575000e-01 5.0094000e-01 /
CHEB / -1.3137000e+00 -4.0886000e-01 1.0765000e-01 /
CHEB / -7.9123000e-01 -7.7363000e-02 -5.3869000e-02 /

CH3CH[OH]CHcH(+m)=CH3+C3H4O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) =
1.5795273369643148 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1924000e+00 7.7759000e-01 -3.5946000e-01 /
CHEB / 9.7195000e+00 1.5246000e+00 1.6472000e-01 /
CHEB / -2.1706000e+00 4.7366000e-01 8.3543000e-02 /
CHEB / -1.3387000e+00 3.9966000e-03 3.7903000e-02 /
CHEB / -7.0244000e-01 -1.2729000e-01 1.5435000e-03 /

CH3CH[OH]CHcH(+m)=CH3+C3H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 1.1995161267318135
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1573000e+00 2.6673000e-01 -1.3178000e-01 /
CHEB / 6.6888000e+00 9.0481000e-01 1.1293000e-01 /
CHEB / -1.9681000e+00 3.2901000e-01 1.4040000e-02 /
CHEB / -1.2020000e+00 3.5850000e-02 1.6379000e-02 /
CHEB / -6.4395000e-01 -8.0592000e-02 1.2253000e-02 /
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```
CH3CH[OH]cCH2(+m)=cH2C[O]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.5274198325402
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2926000e+01 6.3020000e+00 -1.7232000e+00 /
CHEB / 8.4151000e+00 2.3068000e+00 8.3141000e-01 /
CHEB / -3.1446000e+00 -1.0706000e-01 4.4423000e-01 /
CHEB / -1.8347000e+00 -3.9032000e-01 -2.4620000e-02 /
CHEB / -8.6240000e-01 -3.3533000e-01 -8.6072000e-02 /

CH3CH[OH]cCH2(+m)=CH3C[O]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.5274198325402
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3323000e+01 6.2089000e+00 -1.4352000e+00 /
CHEB / 8.7312000e+00 2.1821000e+00 4.8809000e-01 /
CHEB / -3.1286000e+00 -2.9660000e-02 3.8977000e-01 /
CHEB / -1.8254000e+00 -3.3344000e-01 2.7806000e-02 /
CHEB / -8.6100000e-01 -3.2330000e-01 -5.2997000e-02 /

CH3CH[OH]cCH2(+m)=CH3C[O]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.42709102777985
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1373000e+01 6.2123000e+00 -1.1477000e+00 /
CHEB / 7.0701000e+00 1.9092000e+00 3.0771000e-01 /
CHEB / -3.3958000e+00 3.9532000e-02 2.8568000e-01 /
CHEB / -1.8103000e+00 -2.9343000e-01 4.1490000e-02 /
CHEB / -8.3460000e-01 -2.8888000e-01 -3.7057000e-02 /

CH3CH[OH]cCH2(+m)=CH3C[OH]CHcH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    Cd_rad_out_double     Cs_H_out
      deltaHrxn(T=298K) = -28.227161444842416 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1013000e+01 6.7285000e+00 -1.0596000e+00 /
CHEB / 7.6384000e+00 1.5626000e+00 2.2775000e-01 /
CHEB / -3.0985000e+00 3.2431000e-03 2.6504000e-01 /
CHEB / -1.7044000e+00 -2.8309000e-01 5.2664000e-02 /
CHEB / -8.1782000e-01 -2.8356000e-01 -2.6005000e-02 /

CH3CH[OH]cCH2(+m)=CH2C[OH]cHCH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.227161444842416
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0351000e+01 4.5497000e+00 -1.3093000e+00 /
CHEB / 8.1228000e+00 2.7070000e+00 4.4139000e-01 /
CHEB / -2.9775000e+00 2.0344000e-01 3.8957000e-01 /
CHEB / -1.6529000e+00 -2.4834000e-01 3.6015000e-02 /
CHEB / -8.0128000e-01 -2.5437000e-01 -5.2127000e-02 /
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CH3CH[OH]cCH2(+m)=CH2C[OH]CH2cH2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
12.218733803845218 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4418000e+01 6.2620000e+00 -1.8558000e+00 /
CHEB / 8.0268000e+00 2.6777000e+00 9.6037000e-01 /
CHEB / -3.3777000e+00 -3.2252000e-01 5.0423000e-01 /
CHEB / -1.7991000e+00 -6.2340000e-01 -2.8913000e-02 /
CHEB / -7.1977000e-01 -3.8582000e-01 -1.2423000e-01 /

CH3CH[OH]cCH2(+m)=cHC[OH]C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.119832519624607
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5939000e+01 6.1919000e+00 -1.5150000e+00 /
CHEB / 9.1091000e+00 2.1736000e+00 8.9875000e-01 /
CHEB / -2.3514000e+00 -3.8102000e-01 4.0377000e-01 /
CHEB / -1.2635000e+00 -4.1815000e-01 -1.2197000e-02 /
CHEB / -6.1524000e-01 -2.5010000e-01 -7.4018000e-02 /

CH3CH[OH]cCH2(+m)=CH3C[OH]cCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.429348011721016
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3903000e+01 6.0425000e+00 -1.4746000e+00 /
CHEB / 8.3325000e+00 1.9397000e+00 6.4653000e-01 /
CHEB / -2.7441000e+00 -2.4496000e-01 3.2008000e-01 /
CHEB / -1.4757000e+00 -4.2448000e-01 -1.7420000e-04 /
CHEB / -6.7000000e-01 -2.8932000e-01 -7.4004000e-02 /

CH3CH[OH]cCH2(+m)=cH2CH[OH]C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration exact:
Others-R3H_SS    Cd_rad_out_double     Cs_H_out_2H
      deltaHrxn(T=298K) = -7.899125803874433 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.9038000e+00 3.2565000e+00 -9.5839000e-01 /
CHEB / 7.9747000e+00 1.4002000e+00 2.4700000e-01 /
CHEB / -2.8988000e+00 2.0030000e-01 1.6681000e-01 /
CHEB / -1.6214000e+00 -2.2594000e-01 2.8854000e-02 /
CHEB / -7.8433000e-01 -2.5083000e-01 -3.9110000e-02 /

CH3CH[OH]cCH2(+m)=CH3CH[o]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.93938792408224
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2382000e+00 3.6653000e+00 -6.1271000e-01 /
CHEB / 5.0328000e+00 2.8546000e-01 2.9241000e-01 /
CHEB / -3.2142000e+00 -1.6485000e-01 7.5088000e-02 /
CHEB / -1.6402000e+00 -2.7003000e-01 -1.8919000e-02 /
CHEB / -6.7869000e-01 -1.7373000e-01 -3.7789000e-02 /
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CH3CH[OH]cCH2(+m)=CH2CO+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 0.999794344184469
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.1071000e+00 8.9941000e-01 -7.2579000e-01 /
CHEB / 1.1349000e+01 1.9993000e+00 5.1979000e-01 /
CHEB / -1.8462000e+00 3.6786000e-01 1.7583000e-01 /
CHEB / -1.1445000e+00 -1.2672000e-01 -1.1732000e-02 /
CHEB / -5.6347000e-01 -1.4419000e-01 -4.0819000e-02 /

CH3CH[OH]cCH2(+m)=CH3CO+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.049155942531639
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4791000e+00 1.3059000e+00 -5.3389000e-01 /
CHEB / 1.1352000e+01 1.3299000e+00 3.2346000e-01 /
CHEB / -1.8401000e+00 3.0138000e-01 1.1864000e-01 /
CHEB / -1.1305000e+00 -6.2715000e-02 4.6809000e-03 /
CHEB / -5.7071000e-01 -1.1417000e-01 -2.4455000e-02 /

CH3CH[OH]cCH2(+m)=C3H7-1+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.878188626116586
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5612000e+01 1.2772000e+01 1.0466000e-01 /
CHEB / 2.9493000e+01 -1.6131000e+00 6.3189000e-01 /
CHEB / -1.2910000e+00 -1.1580000e+00 3.7410000e-01 /
CHEB / -9.9271000e-01 -5.8325000e-01 1.4973000e-01 /
CHEB / -6.2443000e-01 -1.6532000e-01 1.4850000e-02 /

CH3CH[o]C2H3(+m)=cH2C[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.58803190845796
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4186000e+01 6.7083000e+00 -2.0371000e+00 /
CHEB / 6.4569000e+00 1.5804000e+00 8.0999000e-01 /
CHEB / -3.8809000e+00 -1.4196000e-01 2.5420000e-01 /
CHEB / -2.1061000e+00 -4.2683000e-01 -1.9829000e-02 /
CHEB / -8.8422000e-01 -3.2649000e-01 -6.4050000e-02 /

CH3CH[o]C2H3(+m)=CH3C[O]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.58803190845796
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4383000e+01 6.8361000e+00 -1.7738000e+00 /
CHEB / 6.6456000e+00 1.3460000e+00 5.3146000e-01 /
CHEB / -3.9209000e+00 -1.2894000e-01 2.0664000e-01 /
CHEB / -2.1110000e+00 -4.0486000e-01 6.0870000e-03 /
CHEB / -8.7362000e-01 -3.1071000e-01 -4.5184000e-02 /
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CH3CH[o]C2H3(+m)=CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.48770310369761
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2277000e+01 6.8510000e+00 -1.6615000e+00 /
CHEB / 4.8938000e+00 1.1617000e+00 5.1094000e-01 /
CHEB / -4.2054000e+00 -7.8795000e-02 1.6560000e-01 /
CHEB / -2.0974000e+00 -3.8200000e-01 7.4491000e-03 /
CHEB / -8.4904000e-01 -2.8709000e-01 -4.7331000e-02 /

CH3CH[o]C2H3(+m)=CH3C[OH]CHcH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    O_rad_out     Cs_H_out
      deltaHrxn(T=298K) = -23.287773520760176 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1862000e+01 7.4765000e+00 -1.5212000e+00 /
CHEB / 5.4394000e+00 7.4166000e-01 3.8303000e-01 /
CHEB / -3.8932000e+00 -9.6278000e-02 1.4186000e-01 /
CHEB / -1.9724000e+00 -3.4472000e-01 2.4827000e-02 /
CHEB / -8.2002000e-01 -2.6498000e-01 -3.0427000e-02 /

CH3CH[o]C2H3(+m)=CH2C[OH]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.287773520760176
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1659000e+01 5.0221000e+00 -1.4371000e+00 /
CHEB / 6.2131000e+00 1.9541000e+00 2.7507000e-01 /
CHEB / -3.6771000e+00 1.8352000e-01 1.9781000e-01 /
CHEB / -1.9046000e+00 -2.8615000e-01 3.7090000e-02 /
CHEB / -8.1473000e-01 -2.4894000e-01 -3.5284000e-02 /

CH3CH[o]C2H3(+m)=CH2C[OH]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.279345879762978
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5867000e+01 6.4587000e+00 -2.1607000e+00 /
CHEB / 6.1756000e+00 2.0819000e+00 9.1354000e-01 /
CHEB / -4.0663000e+00 -2.9284000e-01 3.2552000e-01 /
CHEB / -2.0571000e+00 -6.4168000e-01 -2.8205000e-02 /
CHEB / -7.5143000e-01 -3.8677000e-01 -1.1226000e-01 /

CH3CH[o]C2H3(+m)=CH3C[OH]cCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.489960087638776
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4999000e+01 6.3740000e+00 -1.9664000e+00 /
CHEB / 6.2306000e+00 1.3696000e+00 7.9305000e-01 /
CHEB / -3.5543000e+00 -3.0739000e-01 2.2394000e-01 /
CHEB / -1.7658000e+00 -4.9543000e-01 -1.9357000e-02 /
CHEB / -6.9055000e-01 -2.9277000e-01 -8.1367000e-02 /
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```
CH3CH[o]C2H3(+m)=cH2CH[OH]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     Cs_H_out_2H
      deltaHrxn(T=298K) = -2.9597378797921934 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3462000e+01 6.6914000e+00 -7.6785000e-01 /
CHEB / 8.3575000e+00 4.5913000e-01 6.3084000e-02 /
CHEB / -3.4956000e+00 -4.9790000e-01 2.0444000e-01 /
CHEB / -1.9258000e+00 -2.5358000e-01 1.6997000e-03 /
CHEB / -8.2637000e-01 -1.7858000e-01 -4.2785000e-02 /

CH3CH[o]C2H3(+m)=CH3CO+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.1097680184493974
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8944000e+00 2.9733000e+00 -9.5254000e-01 /
CHEB / 8.6815000e+00 7.8926000e-01 6.5399000e-01 /
CHEB / -2.6855000e+00 -5.2739000e-02 1.5301000e-01 /
CHEB / -1.4363000e+00 -2.2174000e-01 -1.9141000e-02 /
CHEB / -5.9630000e-01 -1.3282000e-01 -4.6972000e-02 /

CH3CH[o]C2H3(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.938800702034346
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0225000e+01 1.3756000e+01 -1.0422000e+00 /
CHEB / 3.0278000e+01 -1.8195000e+00 1.0308000e+00 /
CHEB / -2.2989000e+00 -1.1161000e+00 5.8991000e-01 /
CHEB / -1.5619000e+00 -5.4712000e-01 1.1002000e-01 /
CHEB / -8.4651000e-01 -1.2986000e-01 -6.5159000e-02 /

CH2CO+C2H5(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Cd/H2     C_rad/H2/Cs         deltaHrxn(T=298K)
= -26.52721417672467 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7623000e+00 2.0325000e+00 -5.3294000e-01 /
CHEB / -7.0082000e-01 1.4395000e+00 1.3511000e-01 /
CHEB / -2.3717000e+00 2.4325000e-01 2.2316000e-01 /
CHEB / -1.3036000e+00 -1.6264000e-01 7.9670000e-02 /
CHEB / -6.2393000e-01 -1.9833000e-01 -2.0630000e-02 /

CH2CO+C2H5(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -26.52721417672467
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8723000e+00 1.2288000e+00 -6.3185000e-01 /
CHEB / 4.7224000e-02 1.9714000e+00 1.5867000e-01 /
CHEB / -2.2775000e+00 3.9941000e-01 2.3851000e-01 /
CHEB / -1.3292000e+00 -1.5838000e-01 8.5246000e-02 /
CHEB / -6.4807000e-01 -2.1966000e-01 -1.7566000e-02 /
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```
CH2CO+C2H5(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.426885371964318
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6530000e+00 3.8407000e-01 -4.6273000e-01 /
CHEB / 1.2778000e+00 2.5694000e+00 5.8133000e-02 /
CHEB / -2.2610000e+00 6.0393000e-01 1.8111000e-01 /
CHEB / -1.3948000e+00 -1.2720000e-01 6.5502000e-02 /
CHEB / -6.7281000e-01 -2.2267000e-01 -1.6218000e-02 /

CH2CO+C2H5(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.22695578902688
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7873000e+00 -4.0404000e-01 -5.9931000e-01 /
CHEB / 2.6378000e+00 3.2920000e+00 1.7053000e-01 /
CHEB / -1.9818000e+00 6.7832000e-01 2.4037000e-01 /
CHEB / -1.3505000e+00 -1.5160000e-01 6.0193000e-02 /
CHEB / -6.8928000e-01 -2.4491000e-01 -2.6599000e-02 /

CH2CO+C2H5(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.22695578902688
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5453000e+00 1.5082000e-01 -3.0624000e-01 /
CHEB / 3.1656000e+00 2.2227000e+00 5.4505000e-02 /
CHEB / -1.8702000e+00 6.9705000e-01 1.5296000e-01 /
CHEB / -1.2961000e+00 -1.5932000e-02 7.3392000e-02 /
CHEB / -6.7762000e-01 -1.8332000e-01 -5.6604000e-03 /

CH2CO+C2H5(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.218528148029687
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4944000e+00 1.0686000e+00 -6.0026000e-01 /
CHEB / -2.3577000e-01 2.4057000e+00 2.1309000e-01 /
CHEB / -2.5363000e+00 3.4721000e-01 2.6335000e-01 /
CHEB / -1.3710000e+00 -3.1643000e-01 4.7516000e-02 /
CHEB / -5.5138000e-01 -2.9075000e-01 -5.9996000e-02 /

CH2CO+C2H5(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -8.429142355905485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.5548000e-01 -4.0211000e-01 -5.3096000e-01 /
CHEB / 3.3973000e+00 3.1554000e+00 1.9201000e-01 /
CHEB / -1.6987000e+00 4.0503000e-01 2.4331000e-01 /
CHEB / -1.1142000e+00 -2.6328000e-01 1.2764000e-02 /
CHEB / -5.2897000e-01 -2.1770000e-01 -6.0043000e-02 /
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CH2CO+C2H5(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -8.898920148058902
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5862000e+00 5.7350000e-01 -8.6257000e-01 /
CHEB / 8.8187000e+00 2.7780000e+00 4.9737000e-01 /
CHEB / -1.8513000e+00 5.2421000e-01 2.1528000e-01 /
CHEB / -1.2758000e+00 -1.8019000e-01 2.3541000e-02 /
CHEB / -6.5377000e-01 -2.1979000e-01 -4.4358000e-02 /

CH2CO+C2H5(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.939182268266709
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1723000e+01 2.4744000e+00 -1.0345000e+00 /
CHEB / 7.5040000e+00 1.5022000e+00 7.6742000e-01 /
CHEB / -2.3293000e+00 6.9409000e-02 2.0006000e-01 /
CHEB / -1.2961000e+00 -2.4124000e-01 -9.1141000e-03 /
CHEB / -5.4977000e-01 -1.6138000e-01 -5.4711000e-02 /

CH2CO+C2H5(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.048950286716108
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5958000e+00 -1.1402000e+00 -3.5366000e-01 /
CHEB / 3.6376000e+00 1.1900000e+00 2.9419000e-01 /
CHEB / -2.0061000e-01 1.4954000e-01 1.2769000e-01 /
CHEB / -2.2688000e-01 -1.1252000e-01 -6.9780000e-03 /
CHEB / -1.2524000e-01 -8.2156000e-02 -4.0404000e-02 /

CH2CO+C2H5(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -19.877982970301055
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5320000e+01 7.5631000e-05 5.1218000e-05 /
CHEB / 3.0856000e+01 3.6345000e-05 2.7376000e-05 /
CHEB / 4.0418000e-01 -3.6212000e-05 -2.5711000e-05 /
CHEB / 1.1702000e-01 -4.9000000e-05 -3.4345000e-05 /
CHEB / 3.7276000e-02 -2.9489000e-05 -2.0511000e-05 /

CH3CO+C2H4(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -19.478263890008563
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8606000e+00 -1.5141000e-01 -2.4219000e-01 /
CHEB / -2.7716000e-03 1.8830000e+00 7.6656000e-02 /
CHEB / -2.1039000e+00 4.8364000e-01 1.4434000e-01 /
CHEB / -1.3316000e+00 -1.0427000e-01 5.5080000e-02 /
CHEB / -6.5863000e-01 -1.9212000e-01 -1.9946000e-02 /

CH3CO+C2H4(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) CO_rad/NonDe     Cd/H2_Cd/H2
      deltaHrxn(T=298K) = -19.478263890008563 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9265000e+00 9.3876000e-01 -1.2958000e-01 /
CHEB / -1.1018000e+00 8.9125000e-01 6.8812000e-02 /
CHEB / -2.2079000e+00 2.5005000e-01 5.7872000e-02 /
CHEB / -1.2460000e+00 -5.4514000e-02 1.2328000e-02 /
CHEB / -5.9310000e-01 -1.0769000e-01 -1.4559000e-02 /

CH3CO+C2H4(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.37793508524821
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4417000e+00 -5.3103000e-02 -2.0900000e-01 /
CHEB / 1.3844000e+00 1.7479000e+00 1.0531000e-01 /
CHEB / -2.0656000e+00 4.6611000e-01 9.2887000e-02 /
CHEB / -1.3874000e+00 -5.8575000e-02 2.8684000e-02 /
CHEB / -6.8436000e-01 -1.6289000e-01 -1.2288000e-02 /

CH3CO+C2H4(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.178005502310775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9797000e+00 -1.0125000e+00 -3.0279000e-01 /
CHEB / 3.1591000e+00 2.5771000e+00 1.3477000e-01 /
CHEB / -1.8482000e+00 6.2634000e-01 1.4900000e-01 /
CHEB / -1.3748000e+00 -8.0808000e-02 4.7108000e-02 /
CHEB / -7.0039000e-01 -2.0347000e-01 -1.9000000e-02 /

CH3CO+C2H4(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.178005502310775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2070000e+00 -7.7692000e-01 -2.1528000e-01 /
CHEB / 5.6342000e+00 2.3596000e+00 3.0661000e-02 /
CHEB / -1.6109000e+00 5.6974000e-01 1.7026000e-01 /
CHEB / -1.2387000e+00 -1.2748000e-02 4.5512000e-02 /
CHEB / -6.8642000e-01 -1.7144000e-01 -1.6657000e-02 /

CH3CO+C2H4(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.169577861313581
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3563000e+00 -7.5547000e-01 -3.8839000e-01 /
CHEB / 1.5506000e+00 2.6664000e+00 1.9694000e-01 /
CHEB / -2.2608000e+00 4.2999000e-01 2.0894000e-01 /
CHEB / -1.3794000e+00 -2.8260000e-01 3.1253000e-02 /
CHEB / -5.8511000e-01 -2.7165000e-01 -6.0785000e-02 /

CH3CO+C2H4(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -12.829032683584948
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5668000e+01 2.3792000e-06 1.6618000e-06 /
CHEB / 3.2592000e+01 6.1895000e-06 4.3118000e-06 /
CHEB / 2.9021000e-01 1.2383000e-06 8.5682000e-07 /
CHEB / 5.4406000e-02 -2.6555000e-06 -1.8536000e-06 /
CHEB / -2.7904000e-03 -3.2643000e-06 -2.2736000e-06 /

C4H6O(717)+H(+m)=cH2C[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.57664104591231
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6153000e+00 5.5187000e-01 -3.5882000e-01 /
CHEB / -1.1910000e+00 1.7494000e+00 1.4118000e-01 /
CHEB / -2.2367000e+00 6.0188000e-01 1.1848000e-01 /
CHEB / -1.4226000e+00 -3.0240000e-02 5.4299000e-02 /
CHEB / -6.9439000e-01 -2.1114000e-01 -4.1822000e-03 /

C4H6O(717)+H(+m)=CH3C[O]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H/De_Cd/H2     H_rad           deltaHrxn(T=298K) = -
29.57664104591231 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3074000e+00 1.5110000e+00 -1.6786000e-01 /
CHEB / -1.9489000e+00 7.6698000e-01 4.1120000e-02 /
CHEB / -2.3197000e+00 4.2494000e-01 5.6464000e-05 /
CHEB / -1.3506000e+00 5.0481000e-02 2.5898000e-02 /
CHEB / -6.3586000e-01 -1.2336000e-01 2.4657000e-02 /

C4H6O(717)+H(+m)=CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H2_Cd/H/De     H_rad           deltaHrxn(T=298K) = -
32.47631224115196 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1040000e+01 8.9127000e-01 -8.9296000e-02 /
CHEB / -3.4262000e+00 1.3171000e+00 -6.4960000e-02 /
CHEB / -2.5760000e+00 5.2340000e-01 4.8272000e-02 /
CHEB / -1.4274000e+00 4.5747000e-03 4.8342000e-02 /
CHEB / -6.3796000e-01 -1.4542000e-01 4.9937000e-04 /

C4H6O(717)+H(+m)=CH3C[OH]CHcH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad          deltaHrxn(T=298K) = -
32.27638265821452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7891000e+00 -9.2913000e-02 -1.4785000e-01 /
CHEB / -1.7177000e+00 2.1610000e+00 -1.0231000e-01 /
CHEB / -2.2746000e+00 6.9254000e-01 1.2520000e-01 /
CHEB / -1.3833000e+00 -5.2286000e-03 8.5057000e-02 /
CHEB / -6.6220000e-01 -1.9206000e-01 -1.3219000e-02 /
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C4H6O(717)+H(+m)=CH2C[OH]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.27638265821452
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5371000e+00 -9.4292000e-01 -1.1690000e-01 /
CHEB / 1.2646000e+00 2.7713000e+00 -4.1806000e-02 /
CHEB / -1.9016000e+00 6.5965000e-01 1.2938000e-01 /
CHEB / -1.2969000e+00 -1.2976000e-02 5.5678000e-02 /
CHEB / -6.4542000e-01 -1.3719000e-01 -1.4067000e-02 /

C4H6O(717)+H(+m)=CH2C[OH]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.26795501721733
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8433000e+00 -2.3052000e-01 -4.6152000e-01 /
CHEB / -3.6329000e-01 2.7336000e+00 2.2600000e-01 /
CHEB / -2.3624000e+00 5.4359000e-01 1.9903000e-01 /
CHEB / -1.4613000e+00 -2.6659000e-01 3.0427000e-02 /
CHEB / -6.0323000e-01 -2.9907000e-01 -6.1944000e-02 /

C4H6O(717)+H(+m)=cHC[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.169053732996717
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2540000e+00 -1.9646000e-02 -3.9397000e-01 /
CHEB / 1.0662000e+00 2.4035000e+00 3.0545000e-01 /
CHEB / -1.6754000e+00 3.2197000e-01 1.3449000e-01 /
CHEB / -9.9382000e-01 -1.5449000e-01 -1.7549000e-02 /
CHEB / -4.6118000e-01 -1.2514000e-01 -3.0524000e-02 /

C4H6O(717)+H(+m)=CH3C[OH]cCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.478569225093127
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7609000e+00 -1.3185000e-01 -2.0526000e-01 /
CHEB / -3.7276000e-01 2.2319000e+00 -4.7771000e-03 /
CHEB / -2.0127000e+00 4.8926000e-01 1.5410000e-01 /
CHEB / -1.1701000e+00 -1.7381000e-01 3.1739000e-02 /
CHEB / -5.1618000e-01 -1.9190000e-01 -4.7695000e-02 /

C4H6O(717)+H(+m)=cH2CH[OH]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.948347017246544
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.2148000e-01 1.1204000e+00 -6.7726000e-01 /
CHEB / 6.3174000e+00 2.0090000e+00 3.4529000e-01 /
CHEB / -2.1503000e+00 4.7533000e-01 1.5264000e-01 /
CHEB / -1.2787000e+00 -8.8117000e-02 2.5293000e-02 /
CHEB / -6.2721000e-01 -1.6902000e-01 -2.2891000e-02 /
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C4H6O(717)+H(+m)=CH3CH[OH]CHcH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.849445733417678
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5201000e+00 5.4115000e-01 -1.5470000e-01 /
CHEB / 7.4247000e+00 1.3659000e+00 8.0000000e-02 /
CHEB / -1.4674000e+00 5.6824000e-01 6.0430000e-03 /
CHEB / -1.0546000e+00 7.4655000e-02 2.2268000e-02 /
CHEB / -6.5152000e-01 -1.3362000e-01 1.4930000e-02 /

C4H6O(717)+H(+m)=CH3CH[OH]cCH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.04922121337211
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1519000e+00 8.5704000e-01 -1.8467000e-01 /
CHEB / 7.4051000e+00 1.7242000e+00 7.4755000e-02 /
CHEB / -1.4564000e+00 5.4390000e-01 2.8898000e-02 /
CHEB / -1.0091000e+00 -6.1504000e-02 1.8406000e-02 /
CHEB / -5.6013000e-01 -1.7009000e-01 -6.0199000e-03 /

C4H6O(717)+H(+m)=CH3CH[o]C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/Nd/De_O     H_rad       deltaHrxn(T=298K) = -
8.98860913745435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5988000e+00 7.8727000e-01 -1.2547000e-01 /
CHEB / -2.1344000e-02 8.0216000e-01 -3.6004000e-03 /
CHEB / -2.6363000e+00 9.5382000e-02 5.9091000e-02 /
CHEB / -1.3655000e+00 -1.6504000e-01 1.7772000e-02 /
CHEB / -5.5718000e-01 -1.2879000e-01 -1.2653000e-02 /

C4H6O(717)+H(+m)=CH2CO+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.049426869187645
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3936000e+00 -1.3156000e+00 -2.8251000e-01 /
CHEB / 4.2365000e+00 1.3630000e+00 1.9184000e-01 /
CHEB / 5.9393000e-03 1.9568000e-01 1.5041000e-01 /
CHEB / -1.9896000e-01 -1.5312000e-01 8.3895000e-03 /
CHEB / -9.7916000e-02 -1.0119000e-01 -5.0087000e-02 /

C4H6O(717)+H(+m)=CH3CO+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.09837715590375
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1774000e+01 -6.1167000e-01 -1.2454000e-01 /
CHEB / 1.5563000e+00 5.6420000e-01 1.0879000e-01 /
CHEB / -1.5295000e-01 1.7564000e-01 1.6207000e-02 /
CHEB / -1.6283000e-01 -4.9065000e-02 2.2226000e-02 /
CHEB / -7.2482000e-02 -7.5871000e-02 7.3962000e-04 /
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C4H6O(717)+H(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.927409839488696
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0727000e+01 -7.9069000e-05 -5.5069000e-05 /
CHEB / 2.9830000e+01 5.1580000e-05 3.5978000e-05 /
CHEB / 3.9984000e-01 3.9970000e-05 2.7773000e-05 /
CHEB / 1.1379000e-01 3.2427000e-06 2.2486000e-06 /
CHEB / 3.0542000e-02 -8.7649000e-06 -6.0877000e-06 /

C4H6O(717)+H(+m)=CH3+C3H4O-enone(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
0.26991839645336313 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0650000e+01 -8.3946000e-01 -1.4461000e-01 /
CHEB / 2.9423000e+00 9.6831000e-01 1.0153000e-01 /
CHEB / -2.6641000e-01 2.3120000e-02 9.3780000e-02 /
CHEB / -1.1185000e-01 -1.3642000e-01 -2.0356000e-02 /
CHEB / -1.2393000e-03 -4.8918000e-02 -3.6349000e-02 /

C4H6O(717)+H(+m)=CH3+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.6499296066858644
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7189000e+00 -8.3820000e-01 -1.3983000e-01 /
CHEB / 3.9912000e+00 9.2246000e-01 1.0378000e-01 /
CHEB / -6.0534000e-01 6.0560000e-02 7.5515000e-02 /
CHEB / -2.5884000e-01 -1.0914000e-01 -1.4651000e-02 /
CHEB / -3.1424000e-03 -5.7535000e-02 -2.6138000e-02 /

C3H7-1+CO(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.649231206423615
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6218000e+01 1.7282000e+01 -5.2641000e-01 /
CHEB / 3.3113000e+01 -1.7548000e+00 1.6838000e+00 /
CHEB / -1.5002000e+00 -1.8782000e+00 2.9639000e-01 /
CHEB / -1.1243000e+00 -8.0480000e-01 -8.5228000e-03 /
CHEB / -7.5613000e-01 -2.0021000e-01 4.4048000e-02 /

C3H7-1+CO(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: 1,2_Insertion exact:  Cs_Cs
CO_birad          deltaHrxn(T=298K) = -6.649231206423615 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6825000e+01 1.6308000e+01 -2.6227000e-01 /
CHEB / 3.3630000e+01 -1.1159000e+00 1.3799000e+00 /
CHEB / -1.5291000e+00 -1.5283000e+00 1.3908000e-01 /
CHEB / -1.0893000e+00 -8.6119000e-01 9.7060000e-02 /
CHEB / -7.2940000e-01 -2.9232000e-01 1.2420000e-01 /
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C3H7-1+CO(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.548902401663263
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5837000e+01 1.5816000e+01 -3.4858000e-01 /
CHEB / 3.2651000e+01 -9.7060000e-01 1.3321000e+00 /
CHEB / -1.4872000e+00 -1.5941000e+00 4.0539000e-01 /
CHEB / -1.0688000e+00 -6.6392000e-01 7.8328000e-02 /
CHEB / -8.1899000e-01 -6.6030000e-02 -3.0365000e-02 /

C3H7-1+CO(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.348972818725828
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5602000e+01 1.6169000e+01 -3.6436000e-01 /
CHEB / 3.3207000e+01 -1.2691000e+00 1.2828000e+00 /
CHEB / -1.2292000e+00 -1.6983000e+00 3.9606000e-01 /
CHEB / -9.8383000e-01 -6.8390000e-01 8.8819000e-02 /
CHEB / -8.2218000e-01 -3.2413000e-02 -3.8454000e-02 /

C3H7-1+CO(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.348972818725828
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3793000e+01 1.5415000e+01 -3.2812000e-01 /
CHEB / 3.2798000e+01 -1.4037000e+00 1.3808000e+00 /
CHEB / -1.1844000e+00 -1.6253000e+00 4.0228000e-01 /
CHEB / -9.0497000e-01 -5.7738000e-01 7.7943000e-02 /
CHEB / -7.7099000e-01 -6.9671000e-03 -1.0393000e-02 /

CH3+C3H4O-enone(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.306722649458948
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7883000e+00 1.0573000e+00 -5.9540000e-01 /
CHEB / 4.6895000e-01 2.5986000e+00 1.7159000e-01 /
CHEB / -2.5223000e+00 5.2192000e-01 2.1505000e-01 /
CHEB / -1.4966000e+00 -1.8017000e-01 5.8742000e-02 /
CHEB / -6.8220000e-01 -2.4533000e-01 -2.5588000e-02 /

CH3+C3H4O-enone(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
29.306722649458948 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0541000e+00 1.5412000e+00 -4.3954000e-01 /
CHEB / 1.0327000e-01 1.9957000e+00 5.4301000e-02 /
CHEB / -2.5379000e+00 4.7527000e-01 1.2927000e-01 /
CHEB / -1.4637000e+00 -1.3675000e-01 5.4619000e-02 /
CHEB / -6.5825000e-01 -2.0673000e-01 -7.8642000e-03 /

CH3+C3H4O-enone(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) C_methyl     Ck_Cd/H/Nd          deltaHrxn(T=298K)
= -32.206393844698596 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3367000e+00 1.6107000e+00 -2.7724000e-01 /
CHEB / -1.9984000e+00 1.7890000e+00 -5.5881000e-02 /
CHEB / -2.8492000e+00 4.6139000e-01 1.1487000e-01 /
CHEB / -1.4489000e+00 -9.8020000e-02 5.3175000e-02 /
CHEB / -6.2381000e-01 -1.7314000e-01 -1.5577000e-02 /

CH3+C3H4O-enone(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
32.00646426176116 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5266000e+00 7.3714000e-01 -4.9986000e-01 /
CHEB / -5.8454000e-01 2.5216000e+00 4.8199000e-02 /
CHEB / -2.4862000e+00 5.9746000e-01 1.8908000e-01 /
CHEB / -1.3938000e+00 -1.1208000e-01 6.7338000e-02 /
CHEB / -6.5831000e-01 -2.0604000e-01 -1.7055000e-02 /

CH3+C3H4O-enone(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
32.00646426176116 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2477000e+00 -2.9846000e-01 -2.2796000e-01 /
CHEB / 1.7256000e+00 2.7808000e+00 5.6936000e-03 /
CHEB / -2.1053000e+00 6.8646000e-01 1.3962000e-01 /
CHEB / -1.3460000e+00 1.8506000e-02 4.6366000e-02 /
CHEB / -6.7677000e-01 -1.3482000e-01 -1.1103000e-02 /

CH3+C3H4O-enone(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
15.998036620763965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5697000e+00 5.5899000e-01 -7.6082000e-01 /
CHEB / 7.6042000e-01 3.2966000e+00 3.5188000e-01 /
CHEB / -2.6517000e+00 3.8662000e-01 2.7326000e-01 /
CHEB / -1.4876000e+00 -3.6088000e-01 1.2283000e-02 /
CHEB / -5.8363000e-01 -2.9996000e-01 -6.7376000e-02 /

CH3+C3H4O-enone(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.899135336543354
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0009000e-01 6.7993000e-01 -5.9144000e-01 /
CHEB / 1.8586000e+00 2.8880000e+00 4.3214000e-01 /
CHEB / -1.8234000e+00 1.5672000e-01 1.7167000e-01 /
CHEB / -9.9940000e-01 -2.0298000e-01 -2.2896000e-02 /
CHEB / -4.5394000e-01 -1.2178000e-01 -2.6355000e-02 /

CH3+C3H4O-enone(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
11.208650828639763 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0864000e+00 6.2083000e-01 -4.1180000e-01 /
CHEB / 2.6882000e-01 2.4853000e+00 6.1792000e-02 /
CHEB / -2.1481000e+00 3.7940000e-01 2.0003000e-01 /
CHEB / -1.1766000e+00 -2.1681000e-01 2.3855000e-02 /
CHEB / -5.2777000e-01 -1.9006000e-01 -5.1002000e-02 /

CH3+C3H4O-enone(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
11.67842862079318 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1050000e+00 1.1535000e+00 -6.9465000e-01 /
CHEB / 6.1406000e+00 2.2134000e+00 3.7670000e-01 /
CHEB / -2.1849000e+00 4.9701000e-01 1.5617000e-01 /
CHEB / -1.3108000e+00 -9.0431000e-02 2.9236000e-02 /
CHEB / -6.5399000e-01 -1.6809000e-01 -2.0557000e-02 /

CH3+C3H4O-enone(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
3.7793028169187473 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7766000e+00 1.3908000e+00 -5.2885000e-01 /
CHEB / 9.1049000e+00 1.5206000e+00 3.5479000e-01 /
CHEB / -1.9334000e+00 3.4758000e-01 1.2246000e-01 /
CHEB / -1.1018000e+00 -5.3854000e-02 9.3032000e-03 /
CHEB / -5.4313000e-01 -1.0657000e-01 -1.9178000e-02 /

CH3+C3H4O-enone(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
8.718690741000987 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.2043000e+00 3.0863000e+00 -8.7840000e-01 /
CHEB / 4.8291000e+00 9.5275000e-01 6.6317000e-01 /
CHEB / -2.7231000e+00 -2.2232000e-02 1.4549000e-01 /
CHEB / -1.3663000e+00 -2.0079000e-01 -1.9170000e-02 /
CHEB / -5.4605000e-01 -1.1155000e-01 -4.1397000e-02 /

CH3+C3H4O-enone(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.779508472734282
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3358000e+00 -1.4442000e+00 -3.4909000e-01 /
CHEB / 5.4078000e+00 1.6378000e+00 2.9147000e-01 /
CHEB / 3.2433000e-02 2.1242000e-02 1.4166000e-01 /
CHEB / -1.4850000e-01 -1.6898000e-01 -3.7240000e-02 /
CHEB / -6.8175000e-02 -6.3822000e-02 -4.2948000e-02 /

CH3+C3H4O-enone(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.828458759450386
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 7.5282000e+00 -1.0583000e+00 -2.5231000e-01 /
CHEB / 3.8157000e+00 1.1967000e+00 2.1294000e-01 /
CHEB / -2.0076000e-01 4.9466000e-02 1.0375000e-01 /
CHEB / -1.8117000e-01 -1.5390000e-01 -2.3572000e-02 /
CHEB / -6.6550000e-02 -6.3420000e-02 -4.1308000e-02 /

CH3+C3H4O-enone(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.657491443035333
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3371000e+01 -8.3068000e-05 -6.1729000e-05 /
CHEB / 3.0416000e+01 4.9568000e-05 4.0477000e-05 /
CHEB / 5.4192000e-01 1.9109000e-05 1.0776000e-05 /
CHEB / 1.5007000e-01 1.7268000e-05 1.2361000e-05 /
CHEB / 3.3526000e-02 1.3783000e-06 1.1975000e-06 /

C4H6-12+OH(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -57.533885439580494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3304000e+00 5.2811000e+00 -1.3347000e+00 /
CHEB / -3.3803000e+00 2.4042000e+00 9.3119000e-01 /
CHEB / -2.9439000e+00 1.1171000e-01 4.2790000e-01 /
CHEB / -1.5865000e+00 -2.8829000e-01 1.7637000e-02 /
CHEB / -7.1897000e-01 -2.3064000e-01 -7.1243000e-02 /

C4H6-12+OH(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -57.533885439580494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5719000e+00 4.6098000e+00 -1.3208000e+00 /
CHEB / -2.7380000e+00 2.8008000e+00 8.2863000e-01 /
CHEB / -2.8787000e+00 2.7337000e-01 4.2562000e-01 /
CHEB / -1.5966000e+00 -2.6499000e-01 5.3658000e-02 /
CHEB / -7.3309000e-01 -2.4565000e-01 -5.5875000e-02 /

C4H6-12+OH(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -60.43355663482014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9215000e+00 3.9404000e+00 -9.3878000e-01 /
CHEB / -3.9610000e+00 2.9588000e+00 4.3069000e-01 /
CHEB / -3.0557000e+00 5.1792000e-01 3.8732000e-01 /
CHEB / -1.5464000e+00 -1.4678000e-01 1.1165000e-01 /
CHEB / -7.0646000e-01 -1.9471000e-01 -2.9902000e-02 /

C4H6-12+OH(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -60.233627051882706
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0857000e+00 4.1283000e+00 -1.0424000e+00 /
CHEB / -3.2942000e+00 2.8190000e+00 4.9461000e-01 /
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CHEB / -2.8055000e+00 4.3700000e-01 3.7044000e-01 /
CHEB / -1.4804000e+00 -1.8436000e-01 9.6614000e-02 /
CHEB / -7.0487000e-01 -2.0246000e-01 -3.0066000e-02 /

C4H6-12+OH(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ca_Cd/H/Nd     O_pri_rad         deltaHrxn(T=298K)
= -60.233627051882706 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1125000e+00 3.7730000e+00 -7.9907000e-01 /
CHEB / -3.8695000e+00 2.3704000e+00 3.9081000e-01 /
CHEB / -2.7621000e+00 3.7608000e-01 3.7113000e-01 /
CHEB / -1.3884000e+00 -1.2614000e-01 1.1187000e-01 /
CHEB / -6.6671000e-01 -1.3618000e-01 -1.7912000e-02 /

C4H6-12+OH(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -44.22519941088551
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0044000e+00 5.4750000e+00 -1.3444000e+00 /
CHEB / -3.8906000e+00 2.5132000e+00 9.3746000e-01 /
CHEB / -3.1554000e+00 -1.0998000e-01 5.0036000e-01 /
CHEB / -1.5350000e+00 -5.1488000e-01 4.2226000e-02 /
CHEB / -5.7838000e-01 -2.9341000e-01 -9.6018000e-02 /

C4H6-12+OH(+m)=cHC[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.1262981266649
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5089000e-01 5.1539000e+00 -1.0978000e+00 /
CHEB / -2.6578000e+00 2.1923000e+00 1.0285000e+00 /
CHEB / -2.1258000e+00 -2.1500000e-01 4.1429000e-01 /
CHEB / -9.9709000e-01 -3.4079000e-01 5.2298000e-02 /
CHEB / -4.6512000e-01 -1.5661000e-01 -4.9204000e-02 /

C4H6-12+OH(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -39.43581361876131
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3918000e+00 3.9745000e+00 -1.0843000e+00 /
CHEB / -2.6870000e+00 2.9469000e+00 6.3772000e-01 /
CHEB / -2.4307000e+00 1.6564000e-01 3.3883000e-01 /
CHEB / -1.1891000e+00 -3.4446000e-01 4.3137000e-02 /
CHEB / -5.0398000e-01 -2.2755000e-01 -5.2858000e-02 /

C4H6-12+OH(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -39.905591410914724
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9702000e+00 2.3790000e+00 -8.7833000e-01 /
CHEB / -2.8343000e-01 2.3637000e+00 3.6496000e-01 /
CHEB / -2.0391000e+00 2.9697000e-01 2.3198000e-01 /
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CHEB / -1.2750000e+00 -1.9957000e-01 3.7879000e-02 /
CHEB / -6.3547000e-01 -1.9156000e-01 -3.5102000e-02 /

C4H6-12+OH(+m)=CH3CH[OH]CHcH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.80669012708586
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6433000e+00 1.2855000e+00 -5.1703000e-01 /
CHEB / 2.0487000e+00 1.9240000e+00 1.4131000e-01 /
CHEB / -1.8965000e+00 2.7232000e-01 2.1626000e-01 /
CHEB / -1.2971000e+00 -4.0684000e-02 9.1361000e-03 /
CHEB / -6.6684000e-01 -1.6072000e-01 -1.0016000e-02 /

C4H6-12+OH(+m)=CH3CH[OH]cCH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Ca     O_pri_rad         deltaHrxn(T=298K)
= -32.0064656070403 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2506000e+00 1.2995000e+00 -2.4862000e-01 /
CHEB / -1.7022000e+00 1.1054000e+00 7.9072000e-02 /
CHEB / -2.0000000e+00 3.0118000e-01 8.8902000e-02 /
CHEB / -1.1053000e+00 -4.6289000e-02 2.6392000e-02 /
CHEB / -5.5095000e-01 -1.0398000e-01 -1.2400000e-02 /

C4H6-12+OH(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -36.94585353112254
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3595000e-01 3.5613000e+00 -6.5429000e-01 /
CHEB / -2.0067000e+00 7.8821000e-01 2.8695000e-01 /
CHEB / -2.5028000e+00 4.2312000e-02 1.3613000e-01 /
CHEB / -1.3612000e+00 -1.9737000e-01 2.5296000e-02 /
CHEB / -5.9866000e-01 -1.4777000e-01 -2.3565000e-02 /

C4H6-12+OH(+m)=CH2CO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.00667126285582
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4929000e+00 -7.9244000e-01 -3.4361000e-01 /
CHEB / 1.9579000e+00 9.3180000e-01 3.5910000e-01 /
CHEB / -1.0447000e-01 -9.2089000e-03 6.1061000e-02 /
CHEB / -1.1888000e-01 -1.2079000e-01 -5.6502000e-02 /
CHEB / -4.7858000e-02 -3.7054000e-02 -3.3468000e-02 /

C4H6-12+OH(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -38.05562154957193
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0848000e+00 -7.1680000e-01 -3.5682000e-01 /
CHEB / 2.0886000e+00 8.6013000e-01 3.8323000e-01 /
CHEB / -1.7767000e-01 -1.6136000e-02 5.7208000e-02 /
CHEB / -1.5695000e-01 -1.2005000e-01 -6.2481000e-02 /
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CHEB / -6.0628000e-02 -3.8594000e-02 -3.6983000e-02 /

C4H6-12+OH(+m)=C4H6O(717)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.957244393668184
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3647000e+00 -6.5543000e-01 -2.9117000e-01 /
CHEB / 2.1397000e+00 7.8242000e-01 3.0881000e-01 /
CHEB / 7.2459000e-02 -2.2610000e-02 4.6790000e-02 /
CHEB / 1.4096000e-02 -9.9375000e-02 -4.8469000e-02 /
CHEB / 1.7898000e-02 -2.8636000e-02 -2.7776000e-02 /

C4H6-12+OH(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.88465423315688
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4355000e+01 -2.0465000e-02 -1.4679000e-02 /
CHEB / 2.1317000e+01 2.5777000e-02 1.8594000e-02 /
CHEB / 7.6800000e-01 -4.3317000e-03 -3.2651000e-03 /
CHEB / 2.6324000e-01 -8.5530000e-04 -5.7757000e-04 /
CHEB / 8.9427000e-02 -1.9491000e-04 -1.1770000e-04 /

C4H6-12+OH(+m)=CH3+C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.227162790121547
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7582000e+00 -6.7747000e-01 -2.8061000e-01 /
CHEB / 1.7572000e+00 8.1002000e-01 2.9756000e-01 /
CHEB / 1.3856000e-02 -2.7538000e-02 4.4476000e-02 /
CHEB / -6.2855000e-03 -1.0206000e-01 -4.7248000e-02 /
CHEB / 7.1182000e-03 -2.6652000e-02 -2.5838000e-02 /

C4H6-12+OH(+m)=C2H3O-2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.568988045275281
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9083000e+00 -9.2379000e-01 -3.6333000e-01 /
CHEB / 3.2412000e+00 1.1151000e+00 3.8544000e-01 /
CHEB / 1.5939000e-01 -5.8083000e-02 5.7570000e-02 /
CHEB / -7.3405000e-02 -1.3373000e-01 -6.4136000e-02 /
CHEB / -1.6505000e-02 -2.8486000e-02 -3.0480000e-02 /

C4H6-12+OH(+m)=C4H6-2+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.269274969470803
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8821000e+00 -9.3273000e-01 -3.6938000e-01 /
CHEB / 4.0734000e+00 1.1702000e+00 4.1598000e-01 /
CHEB / 4.1285000e-01 -1.2094000e-01 2.7726000e-02 /
CHEB / 3.6151000e-02 -1.3176000e-01 -6.8347000e-02 /
CHEB / 2.8302000e-02 -1.3645000e-02 -2.2230000e-02 /
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C4H6-12+OH(+m)=C2H4O+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.579215516019971
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3800000e+00 -9.8526000e-01 -3.4982000e-01 /
CHEB / 6.4351000e+00 1.1877000e+00 3.6088000e-01 /
CHEB / 6.6419000e-01 -7.6111000e-02 6.2892000e-02 /
CHEB / 7.0406000e-03 -1.1895000e-01 -5.5098000e-02 /
CHEB / -4.6682000e-02 -2.8879000e-02 -2.7230000e-02 /

C4H6-12+OH(+m)=C4H6-13+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -12.018641577000459
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1493000e+00 -1.1477000e+00 -3.6647000e-01 /
CHEB / 3.7960000e+00 1.3357000e+00 3.4813000e-01 /
CHEB / 6.7001000e-02 -1.7812000e-02 1.0250000e-01 /
CHEB / -1.9180000e-01 -1.4177000e-01 -4.7504000e-02 /
CHEB / -1.1641000e-01 -5.0273000e-02 -4.0425000e-02 /

C4H6-12+OH(+m)=C2H5O-2+C2H2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.479350578792186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1677000e+00 -1.0594000e+00 -3.4670000e-01 /
CHEB / 5.5083000e+00 1.1671000e+00 3.3002000e-01 /
CHEB / -6.6865000e-02 6.3761000e-02 8.0549000e-02 /
CHEB / -2.2652000e-01 -1.1965000e-01 -2.5588000e-02 /
CHEB / -1.1664000e-01 -6.1466000e-02 -3.0561000e-02 /

C4H6-12+OH(+m)=nC4H5+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.937782752557993
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9030000e+00 -3.8426000e-01 -2.0793000e-01 /
CHEB / 1.2115000e+01 4.3261000e-01 2.2576000e-01 /
CHEB / 5.4273000e-01 2.0543000e-02 2.0274000e-02 /
CHEB / 7.3200000e-02 -5.8288000e-02 -2.7959000e-02 /
CHEB / -7.9835000e-04 -2.2253000e-02 -1.5129000e-02 /

C4H6-12+OH(+m)=CH3+C3H3OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.819207282092908
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7898000e+00 -7.3981000e-01 -1.6913000e-01 /
CHEB / 2.0619000e+00 8.4112000e-01 1.4194000e-01 /
CHEB / -8.0735000e-02 2.5769000e-02 7.1414000e-02 /
CHEB / -1.2372000e-01 -1.0675000e-01 -1.8496000e-02 /
CHEB / -5.2188000e-02 -4.0374000e-02 -2.7299000e-02 /
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C4H6-12+OH(+m)=CH3+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.60717400035405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9846000e+00 -7.9572000e-01 -1.8649000e-01 /
CHEB / 1.9725000e+00 8.9146000e-01 1.6164000e-01 /
CHEB / 6.8968000e-02 4.1773000e-02 6.5719000e-02 /
CHEB / 4.4298000e-02 -1.0832000e-01 -1.2535000e-02 /
CHEB / 5.4650000e-02 -4.7438000e-02 -2.5947000e-02 /

C4H6-12+OH(+m)=CH3CHO+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.697944372487754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2521000e+00 -7.7342000e-01 -1.9139000e-01 /
CHEB / 2.8732000e+00 8.9772000e-01 1.7671000e-01 /
CHEB / 3.6945000e-01 5.7000000e-05 5.8059000e-02 /
CHEB / 1.4426000e-01 -1.1039000e-01 -2.0520000e-02 /
CHEB / 8.1173000e-02 -3.5085000e-02 -2.5253000e-02 /

C2H3O-2+C2H4(+m)=cH2C[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -49.96489739430521
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0523000e+00 5.0257000e+00 -1.4302000e+00 /
CHEB / -2.9967000e+00 1.5942000e+00 9.7904000e-01 /
CHEB / -2.7960000e+00 1.3284000e-01 3.3499000e-01 /
CHEB / -1.5351000e+00 -2.2193000e-01 -1.2740000e-02 /
CHEB / -7.0528000e-01 -2.3372000e-01 -6.9297000e-02 /

C2H3O-2+C2H4(+m)=CH3C[O]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -49.96489739430521
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2604000e+00 4.3400000e+00 -1.4384000e+00 /
CHEB / -2.3394000e+00 1.9862000e+00 9.0281000e-01 /
CHEB / -2.7182000e+00 3.0058000e-01 3.3069000e-01 /
CHEB / -1.5437000e+00 -1.9178000e-01 1.6435000e-02 /
CHEB / -7.1964000e-01 -2.4787000e-01 -5.2304000e-02 /

C2H3O-2+C2H4(+m)=CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -52.86456858954486
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4993000e+00 2.7875000e+00 -9.4749000e-01 /
CHEB / -2.4333000e+00 3.0334000e+00 4.0800000e-01 /
CHEB / -2.8535000e+00 7.1534000e-01 2.5227000e-01 /
CHEB / -1.5614000e+00 -1.3393000e-01 7.5188000e-02 /
CHEB / -7.2169000e-01 -2.5202000e-01 -1.7028000e-02 /
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C2H3O-2+C2H4(+m)=CH3C[OH]CHcH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -52.66463900660742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2180000e+00 2.3936000e+00 -1.1512000e+00 /
CHEB / -1.3887000e+00 3.4118000e+00 5.2140000e-01 /
CHEB / -2.5908000e+00 7.0141000e-01 2.8133000e-01 /
CHEB / -1.5244000e+00 -1.8400000e-01 6.8979000e-02 /
CHEB / -7.3100000e-01 -2.6443000e-01 -2.3584000e-02 /

C2H3O-2+C2H4(+m)=CH2C[OH]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -52.66463900660742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2166000e+00 2.0925000e+00 -7.6728000e-01 /
CHEB / -1.9145000e+00 2.9606000e+00 2.5158000e-01 /
CHEB / -2.5444000e+00 6.7865000e-01 3.0730000e-01 /
CHEB / -1.4342000e+00 -1.1014000e-01 9.5852000e-02 /
CHEB / -6.9280000e-01 -1.9689000e-01 -2.0803000e-02 /

C2H3O-2+C2H4(+m)=CH2C[OH]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
exact:  Cd_rad/NonDe     Cd/H2_Cd/H2      deltaHrxn(T=298K) = -
36.65621136561023 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4272000e+00 5.6383000e+00 -1.1026000e+00 /
CHEB / -3.8897000e+00 1.0624000e+00 8.3300000e-01 /
CHEB / -3.0748000e+00 -1.4554000e-01 3.7082000e-01 /
CHEB / -1.4869000e+00 -3.7350000e-01 3.9385000e-02 /
CHEB / -5.7640000e-01 -2.2891000e-01 -8.5087000e-02 /

C2H3O-2+C2H4(+m)=cHC[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -26.557310081389616
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0196000e+00 4.5963000e+00 -1.1957000e+00 /
CHEB / -2.1114000e+00 1.5759000e+00 1.1555000e+00 /
CHEB / -2.0353000e+00 -1.1186000e-01 2.7381000e-01 /
CHEB / -1.0027000e+00 -2.3445000e-01 -2.8110000e-02 /
CHEB / -4.7350000e-01 -1.2516000e-01 -6.5967000e-02 /

C2H3O-2+C2H4(+m)=CH3C[OH]cCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.866825573486025
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7649000e+00 2.4596000e+00 -1.2047000e+00 /
CHEB / -9.6300000e-01 3.2404000e+00 6.8893000e-01 /
CHEB / -2.1935000e+00 4.0599000e-01 2.7909000e-01 /
CHEB / -1.2084000e+00 -3.3147000e-01 2.3715000e-02 /
CHEB / -5.3390000e-01 -2.8328000e-01 -4.7641000e-02 /
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C2H3O-2+C2H4(+m)=cH2CH[OH]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.33660336563945
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6206000e-02 9.7233000e-01 -9.8732000e-01 /
CHEB / 2.0356000e+00 3.6821000e+00 6.0317000e-01 /
CHEB / -1.9765000e+00 3.7378000e-01 2.7419000e-01 /
CHEB / -1.3787000e+00 -2.6334000e-01 7.9021000e-03 /
CHEB / -6.5733000e-01 -2.1399000e-01 -5.0180000e-02 /

C2H3O-2+C2H4(+m)=CH3CH[OH]CHcH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.23770208181058
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2032000e+00 2.4725000e-01 -7.1136000e-01 /
CHEB / 4.9453000e+00 2.7442000e+00 5.0019000e-01 /
CHEB / -1.7551000e+00 4.4372000e-01 1.4105000e-01 /
CHEB / -1.3140000e+00 -1.3302000e-01 9.2424000e-04 /
CHEB / -6.7953000e-01 -1.5799000e-01 -1.8677000e-02 /

C2H3O-2+C2H4(+m)=CH3CH[OH]cCH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.43747756176501
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5974000e+00 9.0241000e-01 -8.3159000e-01 /
CHEB / 4.2215000e+00 2.7939000e+00 7.0347000e-01 /
CHEB / -1.7029000e+00 3.2240000e-01 1.7396000e-01 /
CHEB / -1.1288000e+00 -1.8017000e-01 -2.6619000e-02 /
CHEB / -5.3657000e-01 -1.3906000e-01 -3.7967000e-02 /

C2H3O-2+C2H4(+m)=CH3CH[o]C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.37686548584725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3741000e+00 2.7477000e+00 -1.0051000e+00 /
CHEB / 7.7070000e-01 2.3015000e+00 7.6766000e-01 /
CHEB / -2.2068000e+00 -4.6494000e-02 1.7461000e-01 /
CHEB / -1.3085000e+00 -3.3075000e-01 -4.0992000e-02 /
CHEB / -5.6250000e-01 -1.7422000e-01 -7.0736000e-02 /

C2H3O-2+C2H4(+m)=CH2CO+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.437683217580545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0100000e+01 -7.7247000e-01 -3.8306000e-01 /
CHEB / 1.6505000e+00 8.4510000e-01 3.8865000e-01 /
CHEB / -1.9128000e-01 6.1896000e-02 6.6752000e-02 /
CHEB / -1.7184000e-01 -9.9166000e-02 -4.1481000e-02 /
CHEB / -8.0779000e-02 -5.0155000e-02 -3.3943000e-02 /
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C2H3O-2+C2H4(+m)=CH3CO+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.48663350429665
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9062000e+00 -7.0090000e-01 -4.2144000e-01 /
CHEB / 1.6445000e+00 7.8084000e-01 4.4074000e-01 /
CHEB / -3.0751000e-01 6.5539000e-02 7.0779000e-02 /
CHEB / -2.1406000e-01 -1.0557000e-01 -5.1904000e-02 /
CHEB / -9.5981000e-02 -5.9497000e-02 -4.2222000e-02 /

C2H3O-2+C2H4(+m)=C4H6O(717)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -20.388256348392893
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7590000e+00 -9.9630000e-01 -4.7869000e-01 /
CHEB / 3.0369000e+00 1.1020000e+00 4.8869000e-01 /
CHEB / 5.1340000e-02 7.2608000e-02 8.2385000e-02 /
CHEB / -1.1463000e-01 -1.3583000e-01 -5.3135000e-02 /
CHEB / -5.4223000e-02 -6.5475000e-02 -4.3259000e-02 /

C2H3O-2+C2H4(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -43.3156661878816
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6827000e+01 7.1564000e-05 1.3430000e-06 /
CHEB / 2.3646000e+01 -3.7027000e-04 -2.0371000e-04 /
CHEB / 6.7472000e-01 2.0364000e-04 1.4556000e-04 /
CHEB / 2.3976000e-01 1.4226000e-04 9.0356000e-05 /
CHEB / 9.1973000e-02 1.1250000e-05 5.6251000e-06 /

C2H3O-2+C2H4(+m)=CH3+C3H4O-enone(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
20.658174744846264 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9270000e+00 -1.0847000e+00 -4.9247000e-01 /
CHEB / 2.8097000e+00 1.2215000e+00 5.1471000e-01 /
CHEB / 7.0865000e-03 4.2800000e-02 6.5431000e-02 /
CHEB / -1.3844000e-01 -1.4454000e-01 -5.3693000e-02 /
CHEB / -5.9785000e-02 -5.9210000e-02 -3.8904000e-02 /

C2H3O-2+C2H4(+m)=C4H6-13+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.4496535317251755
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6740000e+00 -1.9314000e+00 -6.8854000e-01 /
CHEB / 6.5491000e+00 2.3014000e+00 7.0182000e-01 /
CHEB / 2.1302000e-01 -1.1320000e-01 1.2743000e-01 /
CHEB / -2.6964000e-01 -2.3435000e-01 -9.5907000e-02 /
CHEB / -1.3395000e-01 -5.9434000e-02 -5.6726000e-02 /
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C2H3O-2+C2H4(+m)=nC4H5+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -15.36879470728271
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.6392000e+00 -6.2350000e-01 -3.7256000e-01 /
CHEB / 1.5638000e+01 7.3894000e-01 4.3271000e-01 /
CHEB / 5.8501000e-01 -2.4593000e-02 -3.8037000e-03 /
CHEB / 5.3024000e-02 -8.5178000e-02 -4.9495000e-02 /
CHEB / 5.7786000e-03 -2.1100000e-02 -1.5030000e-02 /

C2H3O-2+C2H4(+m)=CH3+C3H3OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.2502192368176237
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0184000e-01 -1.5117000e+00 -6.1364000e-01 /
CHEB / 8.4759000e+00 1.8511000e+00 6.7544000e-01 /
CHEB / 3.7596000e-01 -1.5821000e-01 4.7528000e-02 /
CHEB / -9.6966000e-02 -1.8483000e-01 -8.9874000e-02 /
CHEB / -5.7299000e-02 -2.6567000e-02 -3.4178000e-02 /

C2H3O-2+C2H4(+m)=CH3+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.038185955078767
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1478000e-01 -1.4338000e+00 -5.6138000e-01 /
CHEB / 5.7627000e+00 1.7101000e+00 5.9650000e-01 /
CHEB / 4.2173000e-01 -8.6415000e-02 6.7230000e-02 /
CHEB / -2.6034000e-02 -1.7337000e-01 -7.0859000e-02 /
CHEB / -5.5061000e-03 -4.7774000e-02 -4.3369000e-02 /

C2H3O-2+C2H4(+m)=CH3CHO+C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.128956327212478
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5494000e+00 -1.3674000e+00 -5.4548000e-01 /
CHEB / 6.7589000e+00 1.6605000e+00 5.9319000e-01 /
CHEB / 6.5358000e-01 -1.2107000e-01 5.1753000e-02 /
CHEB / 4.8281000e-02 -1.6767000e-01 -7.5809000e-02 /
CHEB / 1.8767000e-02 -3.5953000e-02 -3.8349000e-02 /

HCCOH+C2H5(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -60.45363982231012
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3716000e+00 8.0694000e+00 -1.1737000e+00 /
CHEB / -2.7840000e+00 8.4866000e-01 9.8238000e-01 /
CHEB / -2.8358000e+00 -2.5466000e-01 3.6421000e-01 /
CHEB / -1.4593000e+00 -2.9963000e-01 6.4583000e-02 /
CHEB / -6.7556000e-01 -2.0420000e-01 -4.1709000e-02 /
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HCCOH+C2H5(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -60.45363982231012
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1377000e+00 7.3895000e+00 -1.1629000e+00 /
CHEB / -2.1396000e+00 1.2498000e+00 8.8499000e-01 /
CHEB / -2.7675000e+00 -9.0014000e-02 3.6190000e-01 /
CHEB / -1.4681000e+00 -2.7590000e-01 9.8439000e-02 /
CHEB / -6.8930000e-01 -2.1912000e-01 -2.7085000e-02 /

HCCOH+C2H5(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -63.35331101754977
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4438000e+00 5.8615000e+00 -9.4817000e-01 /
CHEB / -2.6764000e+00 2.3427000e+00 6.1640000e-01 /
CHEB / -2.9374000e+00 2.3051000e-01 3.9947000e-01 /
CHEB / -1.4639000e+00 -2.2230000e-01 1.2002000e-01 /
CHEB / -6.8765000e-01 -2.0907000e-01 -2.4656000e-02 /

HCCOH+C2H5(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -63.153381434612335
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5536000e+00 5.6228000e+00 -1.2557000e+00 /
CHEB / -1.7641000e+00 2.6240000e+00 8.5315000e-01 /
CHEB / -2.6842000e+00 1.9074000e-01 4.1861000e-01 /
CHEB / -1.4207000e+00 -2.7447000e-01 9.3962000e-02 /
CHEB / -6.9690000e-01 -2.2086000e-01 -3.9626000e-02 /

HCCOH+C2H5(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -63.153381434612335
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8801000e-01 4.9803000e+00 -1.1604000e+00 /
CHEB / -2.1451000e+00 2.5231000e+00 9.1325000e-01 /
CHEB / -2.6525000e+00 1.3935000e-01 4.2831000e-01 /
CHEB / -1.3472000e+00 -2.3233000e-01 8.7945000e-02 /
CHEB / -6.6132000e-01 -1.5022000e-01 -3.6595000e-02 /

HCCOH+C2H5(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -47.144953793615144
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8044000e+00 7.9802000e+00 -1.3742000e+00 /
CHEB / -3.1299000e+00 1.2071000e+00 1.1984000e+00 /
CHEB / -3.0485000e+00 -4.6587000e-01 4.6311000e-01 /
CHEB / -1.4341000e+00 -5.3143000e-01 6.5228000e-02 /
CHEB / -5.5767000e-01 -2.5913000e-01 -8.6788000e-02 /

HCCOH+C2H5(+m)=cHC[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) Ct/Nd_Ct/H     C_rad/H2/Cs       deltaHrxn(T=298K)
= -37.04605250939453 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2476000e+00 7.8935000e+00 1.1486000e-01 /
CHEB / -2.7687000e+00 -5.0573000e-01 6.3218000e-01 /
CHEB / -2.0340000e+00 -2.5138000e-01 -2.6336000e-02 /
CHEB / -8.8029000e-01 -5.9245000e-02 1.0839000e-01 /
CHEB / -4.1727000e-01 -7.9634000e-02 2.7396000e-02 /

HCCOH+C2H5(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -42.35556800149094
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9342000e+00 5.8571000e+00 -1.1680000e+00 /
CHEB / -1.3888000e+00 2.2857000e+00 8.8006000e-01 /
CHEB / -2.2780000e+00 -1.3100000e-01 3.7155000e-01 /
CHEB / -1.1012000e+00 -4.1998000e-01 6.7766000e-02 /
CHEB / -4.9543000e-01 -2.3786000e-01 -5.2495000e-02 /

HCCOH+C2H5(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -42.82534579364436
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8921000e+00 3.6692000e+00 -1.3787000e+00 /
CHEB / 9.7200000e-01 2.5709000e+00 1.0286000e+00 /
CHEB / -2.0778000e+00 1.7597000e-01 2.9071000e-01 /
CHEB / -1.3083000e+00 -2.5847000e-01 5.4468000e-03 /
CHEB / -6.5706000e-01 -1.8479000e-01 -5.3954000e-02 /

HCCOH+C2H5(+m)=CH3CH[OH]CHcH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.726444509815494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.2638000e+00 1.2438000e+00 -8.1554000e-01 /
CHEB / 2.6697000e+00 2.7246000e+00 5.3635000e-01 /
CHEB / -1.7607000e+00 3.7412000e-01 1.4264000e-01 /
CHEB / -1.2931000e+00 -1.3524000e-01 1.5913000e-02 /
CHEB / -6.8183000e-01 -1.5759000e-01 -1.5384000e-02 /

HCCOH+C2H5(+m)=CH3CH[OH]cCH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.92621998976992
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3475000e+00 2.4727000e+00 -9.1432000e-01 /
CHEB / 2.1287000e+00 2.4431000e+00 8.5158000e-01 /
CHEB / -1.6405000e+00 1.7488000e-01 1.5835000e-01 /
CHEB / -1.0581000e+00 -1.7977000e-01 -2.2608000e-02 /
CHEB / -5.2756000e-01 -1.2451000e-01 -3.5408000e-02 /

HCCOH+C2H5(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -39.86560791385216
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7399000e+00 5.2551000e+00 -1.0456000e+00 /
CHEB / 8.0238000e-01 5.1738000e-01 7.5232000e-01 /
CHEB / -2.1588000e+00 -7.5650000e-02 -1.4462000e-02 /
CHEB / -1.3641000e+00 -9.9717000e-02 -3.9475000e-02 /
CHEB / -6.6168000e-01 -9.0097000e-02 3.0105000e-02 /

HCCOH+C2H5(+m)=CH2CO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -33.926425645585454
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0643000e+00 -2.0879000e-01 -1.4763000e-01 /
CHEB / 2.1070000e+00 2.6206000e-01 1.8261000e-01 /
CHEB / -2.5221000e-01 -3.1557000e-02 -1.7836000e-02 /
CHEB / -1.3570000e-01 -2.2654000e-02 -1.7570000e-02 /
CHEB / -7.8536000e-02 -2.9922000e-03 -2.3920000e-03 /

HCCOH+C2H5(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -40.97537593230156
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4280000e+00 -1.1547000e-01 -1.1314000e-01 /
CHEB / 2.3070000e+00 1.6714000e-01 1.5389000e-01 /
CHEB / -3.0936000e-01 -3.8434000e-02 -2.6014000e-02 /
CHEB / -1.6763000e-01 -1.8464000e-02 -1.7719000e-02 /
CHEB / -8.8944000e-02 -7.0034000e-04 -1.7089000e-03 /

HCCOH+C2H5(+m)=C4H6O(717)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.876998776397805
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5259000e+00 -2.6190000e-01 -1.8405000e-01 /
CHEB / 3.4910000e+00 3.2522000e-01 2.2376000e-01 /
CHEB / 1.6890000e-02 -2.9839000e-02 -1.4459000e-02 /
CHEB / -5.6850000e-02 -3.3640000e-02 -2.4003000e-02 /
CHEB / -4.6630000e-02 -7.2899000e-03 -5.7282000e-03 /

HCCOH+C2H5(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.80440861588651
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5465000e+01 -2.1812000e-02 -1.5418000e-02 /
CHEB / 1.9714000e+01 2.7631000e-02 1.9584000e-02 /
CHEB / 6.2750000e-01 -5.1258000e-03 -3.7048000e-03 /
CHEB / 2.1837000e-01 -4.0043000e-04 -2.5910000e-04 /
CHEB / 7.3522000e-02 -2.8565000e-04 -1.9664000e-04 /

HCCOH+C2H5(+m)=CH3+C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.146917172851175
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 5.9723000e+00 -3.2328000e-01 -2.0690000e-01 /
CHEB / 3.0479000e+00 3.9177000e-01 2.4561000e-01 /
CHEB / -5.6545000e-02 -2.7290000e-02 -1.0521000e-02 /
CHEB / -8.3055000e-02 -3.9336000e-02 -2.5478000e-02 /
CHEB / -5.9104000e-02 -9.3822000e-03 -6.8859000e-03 /

HCCOH+C2H5(+m)=C4H6-12+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.919754382729632
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2152000e+00 -7.1664000e-01 -3.4898000e-01 /
CHEB / 4.6497000e+00 9.1776000e-01 4.1994000e-01 /
CHEB / 3.2611000e-01 -1.2720000e-01 -1.7891000e-02 /
CHEB / -8.0644000e-04 -9.0440000e-02 -5.5720000e-02 /
CHEB / -2.3919000e-02 -7.8266000e-04 -8.7706000e-03 /

HCCOH+C2H5(+m)=C2H3O-2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.48874242800491
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2548000e+00 -5.6962000e-01 -3.2796000e-01 /
CHEB / 3.2874000e+00 6.8844000e-01 3.8359000e-01 /
CHEB / 5.6224000e-02 -4.8442000e-02 -9.3880000e-03 /
CHEB / -4.7821000e-02 -6.6831000e-02 -4.0756000e-02 /
CHEB / -2.7215000e-02 -1.5201000e-02 -1.2093000e-02 /

HCCOH+C2H5(+m)=C4H6-2+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.189029352200432
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1467000e+00 -7.2988000e-01 -3.8941000e-01 /
CHEB / 5.0632000e+00 9.0184000e-01 4.5743000e-01 /
CHEB / 3.6340000e-01 -8.2361000e-02 -7.4589000e-03 /
CHEB / -8.1598000e-04 -9.2199000e-02 -5.5887000e-02 /
CHEB / -1.3845000e-02 -1.7871000e-02 -1.6698000e-02 /

HCCOH+C2H5(+m)=C2H4O+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.498969898749593
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6749000e+00 -1.1675000e+00 -5.5670000e-01 /
CHEB / 7.8557000e+00 1.4480000e+00 6.4436000e-01 /
CHEB / 7.8639000e-01 -1.4965000e-01 -1.4712000e-03 /
CHEB / -1.7130000e-02 -1.3941000e-01 -7.9126000e-02 /
CHEB / -7.5747000e-02 -1.5431000e-02 -2.0834000e-02 /

HCCOH+C2H5(+m)=C4H6-13+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -14.938395959730087
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6965000e-01 -1.1777000e+00 -5.9387000e-01 /
CHEB / 5.5465000e+00 1.4308000e+00 6.7590000e-01 /
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CHEB / 2.3496000e-01 -9.7252000e-02 1.7156000e-02 /
CHEB / -1.8045000e-01 -1.5508000e-01 -8.4540000e-02 /
CHEB / -1.3684000e-01 -2.9245000e-02 -2.9650000e-02 /

HCCOH+C2H5(+m)=C2H5O-2+C2H2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.399104961521822
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2593000e+00 -1.4215000e+00 -5.5758000e-01 /
CHEB / 6.5970000e+00 1.7033000e+00 6.0328000e-01 /
CHEB / 2.9664000e-01 -9.9537000e-02 4.8844000e-02 /
CHEB / -1.9166000e-01 -1.6412000e-01 -6.6537000e-02 /
CHEB / -1.1771000e-01 -4.2984000e-02 -3.3795000e-02 /

HCCOH+C2H5(+m)=nC4H5+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.85753713528762
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7182000e+00 -6.9024000e-01 -3.8779000e-01 /
CHEB / 1.2683000e+01 8.4235000e-01 4.6060000e-01 /
CHEB / 8.0574000e-01 -6.7880000e-02 -2.0951000e-02 /
CHEB / 8.5763000e-02 -8.4053000e-02 -4.7754000e-02 /
CHEB / -1.2947000e-02 -1.4987000e-02 -1.1837000e-02 /

HCCOH+C2H5(+m)=CH3+C3H3OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -12.738961664822536
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2383000e+00 -1.0747000e+00 -5.2870000e-01 /
CHEB / 6.7306000e+00 1.3574000e+00 6.2704000e-01 /
CHEB / 5.6716000e-01 -1.7557000e-01 -2.2715000e-02 /
CHEB / -3.4123000e-02 -1.2181000e-01 -7.4226000e-02 /
CHEB / -7.6895000e-02 -5.3042000e-03 -1.4029000e-02 /

HCCOH+C2H5(+m)=CH3+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.52692838308368
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8631000e+00 -7.9331000e-01 -4.1180000e-01 /
CHEB / 5.0433000e+00 9.6170000e-01 4.7149000e-01 /
CHEB / 4.6318000e-01 -6.9164000e-02 4.6104000e-03 /
CHEB / 3.9110000e-02 -9.8901000e-02 -5.6215000e-02 /
CHEB / -3.2856000e-02 -1.7517000e-02 -1.7861000e-02 /

HCCOH+C2H5(+m)=CH3CHO+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -19.61769875521739
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6766000e-01 -8.0936000e-01 -4.1365000e-01 /
CHEB / 5.8125000e+00 9.9335000e-01 4.7951000e-01 /
CHEB / 6.8917000e-01 -8.7792000e-02 -2.7343000e-03 /
CHEB / 1.0326000e-01 -1.0045000e-01 -5.7821000e-02 /
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CHEB / -1.4605000e-02 -1.3122000e-02 -1.5635000e-02 /

C4H6-1+OH(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -58.58372108399771
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3784000e+00 6.3746000e+00 -1.2567000e+00 /
CHEB / -3.7385000e+00 1.1318000e+00 9.3250000e-01 /
CHEB / -2.5994000e+00 -4.6057000e-02 2.5648000e-01 /
CHEB / -1.3813000e+00 -2.1568000e-01 1.5357000e-02 /
CHEB / -6.3166000e-01 -1.9685000e-01 -3.0949000e-02 /

C4H6-1+OH(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -58.58372108399771
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6058000e+00 5.6944000e+00 -1.2494000e+00 /
CHEB / -3.0899000e+00 1.5319000e+00 8.4170000e-01 /
CHEB / -2.5293000e+00 1.1849000e-01 2.5231000e-01 /
CHEB / -1.3910000e+00 -1.9235000e-01 4.6611000e-02 /
CHEB / -6.4586000e-01 -2.1220000e-01 -1.6509000e-02 /

C4H6-1+OH(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -61.48339227923736
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0917000e+00 4.1096000e+00 -8.4711000e-01 /
CHEB / -3.4202000e+00 2.6652000e+00 3.7571000e-01 /
CHEB / -2.6855000e+00 4.7100000e-01 2.5501000e-01 /
CHEB / -1.4045000e+00 -1.4004000e-01 1.0563000e-01 /
CHEB / -6.4535000e-01 -2.0760000e-01 -4.2957000e-03 /

C4H6-1+OH(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -61.28346269629992
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8495000e+00 3.7128000e+00 -1.1482000e+00 /
CHEB / -2.4082000e+00 3.0460000e+00 5.6466000e-01 /
CHEB / -2.4111000e+00 4.8382000e-01 3.1097000e-01 /
CHEB / -1.3608000e+00 -1.8682000e-01 9.0447000e-02 /
CHEB / -6.6409000e-01 -2.3422000e-01 -2.1623000e-02 /

C4H6-1+OH(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -61.28346269629992
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6503000e+00 3.0431000e+00 -1.0061000e+00 /
CHEB / -2.7270000e+00 2.9995000e+00 5.6420000e-01 /
CHEB / -2.3778000e+00 4.4647000e-01 3.3758000e-01 /
CHEB / -1.2960000e+00 -1.5680000e-01 8.3793000e-02 /
CHEB / -6.3139000e-01 -1.7048000e-01 -2.2711000e-02 /
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C4H6-1+OH(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -45.27503505530272
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8412000e+00 6.0879000e+00 -1.4658000e+00 /
CHEB / -3.9798000e+00 1.6334000e+00 1.1337000e+00 /
CHEB / -2.7991000e+00 -1.9662000e-01 3.7816000e-01 /
CHEB / -1.3664000e+00 -4.4252000e-01 2.4098000e-02 /
CHEB / -5.2288000e-01 -2.5964000e-01 -8.1407000e-02 /

C4H6-1+OH(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ct/Nd_Ct/H     O_pri_rad         deltaHrxn(T=298K)
= -35.176133771082114 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6290000e+00 6.4971000e+00 -1.5135000e-01 /
CHEB / -3.9299000e+00 -2.3207000e-01 7.2506000e-01 /
CHEB / -1.7890000e+00 -3.1106000e-01 -1.2699000e-01 /
CHEB / -7.8135000e-01 -2.3559000e-02 2.6404000e-02 /
CHEB / -3.6094000e-01 -1.1743000e-02 5.2205000e-02 /

C4H6-1+OH(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -40.48564926317852
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4930000e+00 3.9105000e+00 -1.1400000e+00 /
CHEB / -2.0320000e+00 2.7503000e+00 7.0409000e-01 /
CHEB / -2.0080000e+00 1.3996000e-01 2.6644000e-01 /
CHEB / -1.0412000e+00 -3.4353000e-01 5.1335000e-02 /
CHEB / -4.6332000e-01 -2.4501000e-01 -3.6398000e-02 /

C4H6-1+OH(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -40.95542705533194
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4950000e+00 1.8775000e+00 -1.1250000e+00 /
CHEB / 6.6426000e-01 3.2656000e+00 7.5265000e-01 /
CHEB / -1.7503000e+00 3.2579000e-01 2.4080000e-01 /
CHEB / -1.2312000e+00 -2.4586000e-01 1.1949000e-02 /
CHEB / -6.1730000e-01 -2.0716000e-01 -4.4293000e-02 /

C4H6-1+OH(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.856525771503076
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3394000e-01 5.3637000e-01 -6.8742000e-01 /
CHEB / 3.1800000e+00 2.7291000e+00 4.6901000e-01 /
CHEB / -1.4602000e+00 4.1045000e-01 1.2525000e-01 /
CHEB / -1.1947000e+00 -1.2737000e-01 1.2143000e-02 /
CHEB / -6.4617000e-01 -1.5991000e-01 -1.5923000e-02 /
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C4H6-1+OH(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -33.05630125145751
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6228000e-01 1.2845000e+00 -7.9559000e-01 /
CHEB / 2.4341000e+00 2.7644000e+00 6.8953000e-01 /
CHEB / -1.3942000e+00 2.6434000e-01 1.5001000e-01 /
CHEB / -9.8999000e-01 -1.7263000e-01 -1.8247000e-02 /
CHEB / -4.9471000e-01 -1.3438000e-01 -3.3341000e-02 /

C4H6-1+OH(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.99568917553975
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1706000e+00 3.8200000e+00 -1.0861000e+00 /
CHEB / -2.4731000e-01 1.5583000e+00 8.3236000e-01 /
CHEB / -1.8489000e+00 -2.0470000e-01 1.2655000e-01 /
CHEB / -1.1465000e+00 -2.8992000e-01 -6.0551000e-02 /
CHEB / -5.6063000e-01 -1.0042000e-01 -6.3333000e-02 /

C4H6-1+OH(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.05650690727303
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1832000e+01 -3.9773000e-01 -2.3947000e-01 /
CHEB / 9.8829000e-01 4.8167000e-01 2.8132000e-01 /
CHEB / -1.9335000e-02 -3.4986000e-02 -8.5545000e-03 /
CHEB / -6.9796000e-02 -4.6579000e-02 -2.9607000e-02 /
CHEB / -5.4429000e-02 -9.5312000e-03 -7.7298000e-03 /

C4H6-1+OH(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -39.105457193989146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1426000e+01 -3.1132000e-01 -2.3063000e-01 /
CHEB / 1.0608000e+00 3.9579000e-01 2.8116000e-01 /
CHEB / -1.1894000e-01 -3.8922000e-02 -1.3521000e-02 /
CHEB / -1.1267000e-01 -4.5200000e-02 -3.2964000e-02 /
CHEB / -6.6845000e-02 -9.9223000e-03 -9.6908000e-03 /

C4H6-1+OH(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.007080038085398
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0358000e+01 -5.1901000e-01 -3.0951000e-01 /
CHEB / 2.3382000e+00 6.2374000e-01 3.5887000e-01 /
CHEB / 2.2789000e-01 -3.4479000e-02 -3.2475000e-03 /
CHEB / 1.6189000e-03 -6.4838000e-02 -3.8357000e-02 /
CHEB / -2.2851000e-02 -1.6119000e-02 -1.2939000e-02 /
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C4H6-1+OH(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.934489877574094
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3140000e+01 -1.3805000e-02 -9.9016000e-03 /
CHEB / 2.1015000e+01 1.7598000e-02 1.2699000e-02 /
CHEB / 7.2451000e-01 -3.4369000e-03 -2.5922000e-03 /
CHEB / 2.4514000e-01 -8.9731000e-05 -1.3111000e-05 /
CHEB / 8.5854000e-02 -2.5008000e-04 -1.8068000e-04 /

C4H6-1+OH(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.27699843453876
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0649000e+01 -5.9483000e-01 -3.3127000e-01 /
CHEB / 1.9948000e+00 7.1245000e-01 3.8403000e-01 /
CHEB / 1.7430000e-01 -4.0882000e-02 -6.4157000e-03 /
CHEB / -2.2299000e-02 -7.1241000e-02 -3.9013000e-02 /
CHEB / -3.5569000e-02 -1.6432000e-02 -1.2124000e-02 /

C4H6-1+OH(+m)=C4H6-12+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.049835644417218
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9520000e+00 -9.1521000e-01 -3.9190000e-01 /
CHEB / 4.5620000e+00 1.1575000e+00 4.5397000e-01 /
CHEB / 4.9946000e-01 -1.4082000e-01 5.8287000e-03 /
CHEB / 3.9210000e-02 -1.1659000e-01 -6.4808000e-02 /
CHEB / -5.8880000e-03 -8.5365000e-03 -1.6804000e-02 /

C4H6-1+OH(+m)=C2H3O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -8.618823689692496
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4812000e+00 -8.1996000e-01 -4.1623000e-01 /
CHEB / 2.6836000e+00 9.8675000e-01 4.7481000e-01 /
CHEB / 3.0159000e-01 -6.7478000e-02 2.8120000e-03 /
CHEB / -1.5942000e-02 -9.1457000e-02 -5.0300000e-02 /
CHEB / -1.5424000e-02 -2.2393000e-02 -1.7972000e-02 /

C4H6-1+OH(+m)=HCCOH+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = 1.869918738312414
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1663000e+00 -1.3459000e-01 -8.0976000e-02 /
CHEB / 4.1305000e+00 1.8891000e-01 1.1094000e-01 /
CHEB / 3.1164000e-01 -5.2184000e-02 -2.5940000e-02 /
CHEB / 5.8969000e-02 -7.9900000e-03 -8.0947000e-03 /
CHEB / -8.1367000e-03 5.0709000e-03 3.2193000e-03 /
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C4H6-1+OH(+m)=C4H6-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.319110613888018
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3932000e+00 -1.0272000e+00 -4.9397000e-01 /
CHEB / 4.4464000e+00 1.2509000e+00 5.6699000e-01 /
CHEB / 6.1993000e-01 -9.8135000e-02 1.9137000e-03 /
CHEB / 3.7633000e-02 -1.1981000e-01 -6.1689000e-02 /
CHEB / -6.6763000e-03 -2.8686000e-02 -2.3842000e-02 /

C4H6-1+OH(+m)=C2H4O+C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.629051160437186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8581000e+00 -1.3892000e+00 -5.9407000e-01 /
CHEB / 8.0000000e+00 1.7093000e+00 6.6586000e-01 /
CHEB / 9.8231000e-01 -1.6063000e-01 2.8156000e-02 /
CHEB / 2.0251000e-02 -1.6323000e-01 -8.4734000e-02 /
CHEB / -6.0879000e-02 -2.4671000e-02 -2.9694000e-02 /

C4H6-1+OH(+m)=C4H6-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.068477221417673
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6717000e+00 -1.5955000e+00 -6.5631000e-01 /
CHEB / 5.2232000e+00 1.9207000e+00 7.0961000e-01 /
CHEB / 4.9265000e-01 -1.1770000e-01 6.4721000e-02 /
CHEB / -1.4302000e-01 -1.9522000e-01 -8.6510000e-02 /
CHEB / -1.2343000e-01 -4.6079000e-02 -4.4826000e-02 /

C4H6-1+OH(+m)=C2H5O-2+C2H2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -7.5291862232094005
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1667000e+00 -1.6447000e+00 -5.4909000e-01 /
CHEB / 6.9247000e+00 1.9242000e+00 5.6417000e-01 /
CHEB / 4.3357000e-01 -5.7538000e-02 7.9587000e-02 /
CHEB / -1.6542000e-01 -1.8480000e-01 -5.4690000e-02 /
CHEB / -1.0926000e-01 -5.9647000e-02 -3.8830000e-02 /

C4H6-1+OH(+m)=nC4H5+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.987618396975208
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0163000e+00 -6.5830000e-01 -3.7856000e-01 /
CHEB / 1.3717000e+01 7.9225000e-01 4.4471000e-01 /
CHEB / 8.6159000e-01 -4.8309000e-02 -1.3588000e-02 /
CHEB / 1.1637000e-01 -8.1285000e-02 -4.6370000e-02 /
CHEB / 1.7254000e-03 -1.8799000e-02 -1.3529000e-02 /
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C4H6-1+OH(+m)=CH3+C3H3OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.869042926510122
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3265000e+00 -1.3353000e+00 -5.6763000e-01 /
CHEB / 6.8933000e+00 1.6657000e+00 6.4499000e-01 /
CHEB / 7.1304000e-01 -1.8719000e-01 1.5811000e-02 /
CHEB / 5.0603000e-03 -1.5438000e-01 -8.2287000e-02 /
CHEB / -5.7079000e-02 -1.4996000e-02 -2.5167000e-02 /

C4H6-1+OH(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.657009644771264
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2627000e+00 -1.1168000e+00 -4.9941000e-01 /
CHEB / 4.5106000e+00 1.3508000e+00 5.5883000e-01 /
CHEB / 7.0274000e-01 -9.7579000e-02 1.8840000e-02 /
CHEB / 9.1442000e-02 -1.2872000e-01 -5.9735000e-02 /
CHEB / -7.0853000e-03 -3.0516000e-02 -2.8534000e-02 /

C4H6-1+OH(+m)=CH3CHO+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -17.74778001690497
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5833000e+00 -1.0940000e+00 -4.8866000e-01 /
CHEB / 5.4305000e+00 1.3445000e+00 5.5574000e-01 /
CHEB / 9.3381000e-01 -1.2433000e-01 9.0647000e-03 /
CHEB / 1.5375000e-01 -1.2664000e-01 -6.2538000e-02 /
CHEB / 1.0174000e-02 -2.2986000e-02 -2.5337000e-02 /

C4H6-2+OH(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.264610470109695
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0876000e+00 3.3726000e+00 -1.4176000e+00 /
CHEB / -1.8554000e+00 2.4252000e+00 7.5136000e-01 /
CHEB / -2.3525000e+00 2.3624000e-01 2.7594000e-01 /
CHEB / -1.4684000e+00 -2.5046000e-01 5.6220000e-03 /
CHEB / -7.0633000e-01 -2.6297000e-01 -5.4859000e-02 /

C4H6-2+OH(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.264610470109695
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9842000e+00 3.4958000e+00 -1.1789000e+00 /
CHEB / -1.7962000e+00 2.1931000e+00 4.8567000e-01 /
CHEB / -2.3826000e+00 2.2710000e-01 2.4778000e-01 /
CHEB / -1.4619000e+00 -2.2739000e-01 2.2007000e-02 /
CHEB / -6.9529000e-01 -2.4575000e-01 -4.2717000e-02 /
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C4H6-2+OH(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -54.16428166534934
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1475000e+00 3.4105000e+00 -1.0907000e+00 /
CHEB / -3.7357000e+00 2.1592000e+00 4.6603000e-01 /
CHEB / -2.6780000e+00 2.2572000e-01 2.2382000e-01 /
CHEB / -1.4603000e+00 -2.0381000e-01 5.9348000e-03 /
CHEB / -6.7077000e-01 -2.1610000e-01 -5.1335000e-02 /

C4H6-2+OH(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.96435208241191
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6400000e+00 2.8673000e+00 -1.3141000e+00 /
CHEB / -2.6335000e+00 2.5425000e+00 5.9420000e-01 /
CHEB / -2.3432000e+00 3.1533000e-01 2.5764000e-01 /
CHEB / -1.3784000e+00 -1.8528000e-01 1.5878000e-02 /
CHEB / -6.8045000e-01 -2.2149000e-01 -4.3245000e-02 /

C4H6-2+OH(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.96435208241191
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7270000e+00 1.2216000e+00 -8.6025000e-01 /
CHEB / -1.5189000e+00 3.2215000e+00 2.7728000e-01 /
CHEB / -2.1558000e+00 6.1825000e-01 2.1070000e-01 /
CHEB / -1.3147000e+00 -1.3155000e-01 4.2435000e-02 /
CHEB / -6.5712000e-01 -1.9444000e-01 -2.3863000e-02 /

C4H6-2+OH(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.95592444141471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2580000e+00 3.1036000e+00 -1.5924000e+00 /
CHEB / -1.9592000e+00 2.9167000e+00 9.5195000e-01 /
CHEB / -2.5089000e+00 8.2910000e-02 3.2810000e-01 /
CHEB / -1.4396000e+00 -4.5706000e-01 -2.8383000e-02 /
CHEB / -5.8956000e-01 -3.1954000e-01 -9.9402000e-02 /

C4H6-2+OH(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.8570231571941
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8938000e+00 3.1989000e+00 -1.3071000e+00 /
CHEB / -9.4082000e-01 2.3756000e+00 9.5657000e-01 /
CHEB / -1.5674000e+00 -8.5878000e-02 2.1326000e-01 /
CHEB / -9.1969000e-01 -2.6996000e-01 -2.0221000e-02 /
CHEB / -4.7120000e-01 -1.5297000e-01 -4.6412000e-02 /

C4H6-2+OH(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) Ct/Nd_Ct/Nd     O_pri_rad        deltaHrxn(T=298K)
= -33.16653864929051 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9578000e+00 3.9256000e+00 -9.3429000e-01 /
CHEB / -3.0325000e+00 1.2708000e+00 4.6344000e-01 /
CHEB / -1.9070000e+00 -1.1388000e-01 2.5629000e-01 /
CHEB / -1.0438000e+00 -2.4116000e-01 1.0729000e-02 /
CHEB / -5.1567000e-01 -1.4411000e-01 -6.4871000e-02 /

C4H6-2+OH(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -33.636316441443924
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0055000e+00 1.0640000e+00 -8.7255000e-01 /
CHEB / 1.0751000e+00 3.0488000e+00 5.6747000e-01 /
CHEB / -1.8152000e+00 4.2053000e-01 2.1026000e-01 /
CHEB / -1.2714000e+00 -1.6567000e-01 2.1942000e-02 /
CHEB / -6.4637000e-01 -1.8674000e-01 -3.0737000e-02 /

C4H6-2+OH(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.53741515761506
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7636000e-01 5.6619000e-01 -5.3698000e-01 /
CHEB / 4.2980000e+00 2.1996000e+00 3.9338000e-01 /
CHEB / -1.5696000e+00 4.9012000e-01 1.0402000e-01 /
CHEB / -1.2024000e+00 -4.8447000e-02 1.7882000e-02 /
CHEB / -6.6871000e-01 -1.4272000e-01 -1.0307000e-02 /

C4H6-2+OH(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.737190637569494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0401000e+00 1.1690000e+00 -6.9171000e-01 /
CHEB / 3.5704000e+00 2.1921000e+00 5.9830000e-01 /
CHEB / -1.5541000e+00 3.4913000e-01 1.4381000e-01 /
CHEB / -1.0401000e+00 -9.7752000e-02 -7.0724000e-03 /
CHEB / -5.2884000e-01 -1.1448000e-01 -2.6042000e-02 /

C4H6-2+OH(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.676578561651734
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2649000e+00 2.9231000e+00 -9.6675000e-01 /
CHEB / -2.6590000e-01 1.7205000e+00 8.0312000e-01 /
CHEB / -2.2103000e+00 -3.9648000e-02 1.4904000e-01 /
CHEB / -1.2525000e+00 -2.4182000e-01 -3.8126000e-02 /
CHEB / -5.3255000e-01 -1.3130000e-01 -5.6059000e-02 /

C4H6-2+OH(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.73739629338502
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0922000e+00 -1.2392000e+00 -5.3474000e-01 /
CHEB / 2.6386000e+00 1.4013000e+00 5.5155000e-01 /
CHEB / 1.2005000e-01 2.7779000e-02 7.8746000e-02 /
CHEB / -1.5579000e-01 -1.4600000e-01 -5.7061000e-02 /
CHEB / -9.6026000e-02 -6.2989000e-02 -4.0123000e-02 /

C4H6-2+OH(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.78634658010113
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0215000e+01 -7.7004000e-01 -4.1381000e-01 /
CHEB / 1.8396000e+00 8.9759000e-01 4.4159000e-01 /
CHEB / -2.1445000e-01 6.0818000e-03 5.7503000e-02 /
CHEB / -2.8596000e-01 -1.0627000e-01 -5.5898000e-02 /
CHEB / -1.5119000e-01 -4.7396000e-02 -3.5391000e-02 /

C4H6-2+OH(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.687969424197384
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1212000e+01 -7.5002000e-01 -3.7215000e-01 /
CHEB / 1.2779000e+00 8.7674000e-01 3.9891000e-01 /
CHEB / -1.4501000e-01 -7.0142000e-03 4.6728000e-02 /
CHEB / -1.5370000e-01 -1.0159000e-01 -5.2162000e-02 /
CHEB / -4.9849000e-02 -3.9430000e-02 -2.9887000e-02 /

C4H6-2+OH(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -44.61537926368608
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7345000e+01 -8.2724000e-05 -2.8430000e-04 /
CHEB / 2.4379000e+01 2.9615000e-04 5.7537000e-04 /
CHEB / 8.5906000e-01 -5.4897000e-04 -5.7771000e-04 /
CHEB / 2.4189000e-01 4.4727000e-04 3.7183000e-04 /
CHEB / 6.6708000e-02 -5.9454000e-05 -4.5583000e-05 /

C4H6-2+OH(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.957887820650747
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1374000e+01 -7.7883000e-01 -3.5355000e-01 /
CHEB / 9.9563000e-01 9.1256000e-01 3.7894000e-01 /
CHEB / -1.9283000e-01 -1.7105000e-02 4.2070000e-02 /
CHEB / -1.7903000e-01 -1.0189000e-01 -4.9297000e-02 /
CHEB / -6.1204000e-02 -3.4275000e-02 -2.6039000e-02 /

C4H6-2+OH(+m)=C2H3O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.2997130758044815
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 6.2119000e+00 -1.4478000e+00 -5.9611000e-01 /
CHEB / 5.1886000e+00 1.7331000e+00 6.4970000e-01 /
CHEB / 3.6025000e-01 -8.6751000e-02 5.3853000e-02 /
CHEB / -1.5672000e-01 -1.8656000e-01 -8.1392000e-02 /
CHEB / -6.8729000e-02 -4.8861000e-02 -4.0650000e-02 /

C4H6-2+OH(+m)=C2H4O+C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.30994054654917136
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0511000e+00 -1.2151000e+00 -5.2289000e-01 /
CHEB / 8.9418000e+00 1.4739000e+00 5.8518000e-01 /
CHEB / 1.0101000e+00 -1.0082000e-01 2.6901000e-02 /
CHEB / 1.0422000e-01 -1.5446000e-01 -7.2654000e-02 /
CHEB / -2.9839000e-02 -3.3704000e-02 -2.9913000e-02 /

C4H6-2+OH(+m)=C4H6-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.749366607529659
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3623000e+00 -1.6305000e+00 -5.9744000e-01 /
CHEB / 5.5915000e+00 1.9294000e+00 6.2439000e-01 /
CHEB / 5.2227000e-01 -7.1946000e-02 8.7146000e-02 /
CHEB / -6.7082000e-02 -1.9576000e-01 -7.4493000e-02 /
CHEB / -8.0101000e-02 -6.5847000e-02 -4.8511000e-02 /

C4H6-2+OH(+m)=C2H5O-2+C2H2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.21007560932138603
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2607000e-01 -1.4715000e+00 -4.3696000e-01 /
CHEB / 8.0482000e+00 1.6564000e+00 4.3591000e-01 /
CHEB / 4.2615000e-01 4.0105000e-02 7.1328000e-02 /
CHEB / -1.0302000e-01 -1.6519000e-01 -2.8370000e-02 /
CHEB / -8.1697000e-02 -7.8090000e-02 -3.3333000e-02 /

C4H6-2+OH(+m)=nC4H5+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.668507783087193
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.4883000e+00 -4.5998000e-01 -2.6613000e-01 /
CHEB / 1.5496000e+01 5.3164000e-01 3.0181000e-01 /
CHEB / 8.7272000e-01 9.0595000e-04 5.8911000e-03 /
CHEB / 1.6173000e-01 -6.2965000e-02 -3.2640000e-02 /
CHEB / 1.8971000e-02 -2.1726000e-02 -1.4403000e-02 /

C4H6-2+OH(+m)=CH3+C3H3OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.549932312622107
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4957000e+00 -1.1754000e+00 -4.8698000e-01 /
CHEB / 7.9057000e+00 1.4414000e+00 5.4926000e-01 /
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CHEB / 6.7865000e-01 -1.1600000e-01 2.0763000e-02 /
CHEB / 7.9597000e-02 -1.5368000e-01 -6.9182000e-02 /
CHEB / -1.6123000e-02 -2.6253000e-02 -2.7262000e-02 /

C4H6-2+OH(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.33789903088325
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0992000e+00 -1.0687000e+00 -4.9600000e-01 /
CHEB / 4.7627000e+00 1.2955000e+00 5.6370000e-01 /
CHEB / 6.9976000e-01 -9.5015000e-02 1.0692000e-02 /
CHEB / 2.0474000e-01 -1.2069000e-01 -6.2590000e-02 /
CHEB / 6.9120000e-02 -3.4077000e-02 -2.6655000e-02 /

C4H6-2+OH(+m)=CH3CHO+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.428669403016968
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2531000e+00 -1.0075000e+00 -4.6980000e-01 /
CHEB / 5.8404000e+00 1.2493000e+00 5.4697000e-01 /
CHEB / 9.7938000e-01 -1.2690000e-01 -4.9485000e-03 /
CHEB / 2.7489000e-01 -1.1459000e-01 -6.2932000e-02 /
CHEB / 7.7270000e-02 -2.4640000e-02 -2.2137000e-02 /

C2H4O+C2H3(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.95466992356052
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0524000e+00 4.9453000e+00 -1.5946000e+00 /
CHEB / 2.4735000e+00 3.1767000e+00 1.0773000e+00 /
CHEB / -2.1218000e+00 1.7633000e-01 4.5422000e-01 /
CHEB / -1.4101000e+00 -3.6638000e-01 1.4300000e-02 /
CHEB / -6.8784000e-01 -2.8852000e-01 -7.2974000e-02 /

C2H4O+C2H3(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.95466992356052
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4553000e+00 4.8278000e+00 -1.3396000e+00 /
CHEB / 2.7629000e+00 3.0239000e+00 7.4231000e-01 /
CHEB / -2.0765000e+00 2.9981000e-01 4.1796000e-01 /
CHEB / -1.3926000e+00 -2.9533000e-01 7.6683000e-02 /
CHEB / -6.9265000e-01 -2.8613000e-01 -4.2640000e-02 /

C2H4O+C2H3(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.85434111880017
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4846000e+00 4.8188000e+00 -1.1143000e+00 /
CHEB / 1.0594000e+00 2.7350000e+00 6.1871000e-01 /
CHEB / -2.3430000e+00 3.7490000e-01 3.1451000e-01 /
CHEB / -1.3663000e+00 -2.4708000e-01 8.4803000e-02 /
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CHEB / -6.6414000e-01 -2.4636000e-01 -2.4108000e-02 /

C2H4O+C2H3(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.654411535862735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1256000e+00 5.3341000e+00 -1.0268000e+00 /
CHEB / 1.6153000e+00 2.3683000e+00 5.2732000e-01 /
CHEB / -2.0470000e+00 3.3610000e-01 2.9343000e-01 /
CHEB / -1.2659000e+00 -2.4447000e-01 9.1200000e-02 /
CHEB / -6.5159000e-01 -2.4756000e-01 -1.6670000e-02 /

C2H4O+C2H3(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.654411535862735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4883000e+00 3.1812000e+00 -1.1751000e+00 /
CHEB / 2.1762000e+00 3.5591000e+00 6.6597000e-01 /
CHEB / -1.9563000e+00 4.8633000e-01 4.0551000e-01 /
CHEB / -1.2239000e+00 -2.1640000e-01 7.2932000e-02 /
CHEB / -6.2685000e-01 -2.0096000e-01 -4.1126000e-02 /

C2H4O+C2H3(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.64598389486554
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5266000e+00 4.9397000e+00 -1.6974000e+00 /
CHEB / 2.0962000e+00 3.5547000e+00 1.2013000e+00 /
CHEB / -2.3826000e+00 -8.8025000e-02 4.9589000e-01 /
CHEB / -1.3721000e+00 -6.0173000e-01 6.5336000e-03 /
CHEB / -5.3750000e-01 -3.2831000e-01 -1.0535000e-01 /

C2H4O+C2H3(+m)=cHC[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.547082610644928
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0549000e+00 4.8290000e+00 -1.3651000e+00 /
CHEB / 3.1812000e+00 3.0189000e+00 1.1575000e+00 /
CHEB / -1.3293000e+00 -1.2870000e-01 4.1572000e-01 /
CHEB / -8.3022000e-01 -3.9087000e-01 3.4542000e-02 /
CHEB / -4.3948000e-01 -1.9983000e-01 -6.0134000e-02 /

C2H4O+C2H3(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.85659810274134
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0174000e+00 4.6688000e+00 -1.4000000e+00 /
CHEB / 2.3613000e+00 2.7935000e+00 9.3776000e-01 /
CHEB / -1.7186000e+00 5.9442000e-02 3.3207000e-01 /
CHEB / -1.0324000e+00 -3.8866000e-01 3.9595000e-02 /
CHEB / -4.9330000e-01 -2.3968000e-01 -5.8123000e-02 /
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C2H4O+C2H3(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     Cd_pri_rad
      deltaHrxn(T=298K) = -33.32637589489475 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0718000e+00 2.8307000e+00 -7.3148000e-01 /
CHEB / 9.7225000e-01 1.4476000e+00 2.5090000e-01 /
CHEB / -2.0246000e+00 3.5401000e-01 1.9051000e-01 /
CHEB / -1.1749000e+00 -8.1905000e-02 5.9280000e-02 /
CHEB / -5.9530000e-01 -1.5724000e-01 -1.8209000e-02 /

C2H4O+C2H3(+m)=CH3CH[OH]CHcH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.22747461106589
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6724000e-01 6.5582000e-01 -4.0595000e-01 /
CHEB / 4.4767000e+00 2.0972000e+00 1.4677000e-01 /
CHEB / -1.4218000e+00 4.9680000e-01 1.5796000e-01 /
CHEB / -1.1543000e+00 -8.3812000e-02 4.4663000e-02 /
CHEB / -6.3928000e-01 -1.7472000e-01 -1.9054000e-02 /

C2H4O+C2H3(+m)=CH3CH[OH]cCH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.427250091020323
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5132000e-01 1.3134000e+00 -4.8581000e-01 /
CHEB / 3.7430000e+00 2.2073000e+00 2.7377000e-01 /
CHEB / -1.4216000e+00 3.0977000e-01 1.7725000e-01 /
CHEB / -9.9414000e-01 -1.4509000e-01 1.4021000e-02 /
CHEB / -5.0620000e-01 -1.4536000e-01 -3.4612000e-02 /

C2H4O+C2H3(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.366638015102563
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5479000e+00 4.3445000e+00 -4.2078000e-01 /
CHEB / 3.1264000e+00 2.7786000e-01 1.0254000e-01 /
CHEB / -1.8789000e+00 5.3444000e-02 -9.1408000e-04 /
CHEB / -1.2550000e+00 -6.5197000e-02 5.5007000e-02 /
CHEB / -6.2495000e-01 -1.1034000e-01 4.1345000e-02 /

C2H4O+C2H3(+m)=CH2CO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.42745574683585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2193000e+00 -1.3275000e+00 -5.5234000e-01 /
CHEB / 7.7841000e+00 1.5400000e+00 5.7155000e-01 /
CHEB / 5.0286000e-01 -6.3091000e-03 9.1824000e-02 /
CHEB / -1.1299000e-01 -1.8174000e-01 -7.5332000e-02 /
CHEB / -1.0561000e-01 -5.6910000e-02 -4.7841000e-02 /
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C2H4O+C2H3(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.47640603355196
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5796000e+00 -8.7011000e-01 -3.9051000e-01 /
CHEB / 7.4108000e+00 9.9450000e-01 4.0869000e-01 /
CHEB / 4.3194000e-01 2.0677000e-02 5.7323000e-02 /
CHEB / -1.1712000e-01 -1.1376000e-01 -4.3946000e-02 /
CHEB / -1.2293000e-01 -4.8559000e-02 -3.4462000e-02 /

C2H4O+C2H3(+m)=C4H6O(717)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.378028877648212
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8171000e+00 -8.5092000e-01 -3.6882000e-01 /
CHEB / 6.8985000e+00 9.7148000e-01 3.8498000e-01 /
CHEB / 5.2367000e-01 1.1931000e-02 5.0635000e-02 /
CHEB / -1.3584000e-03 -1.0805000e-01 -4.1569000e-02 /
CHEB / -5.1602000e-02 -4.0861000e-02 -2.8931000e-02 /

C2H4O+C2H3(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -44.30543871713691
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0875000e+01 -5.8597000e-02 -4.2129000e-02 /
CHEB / 2.5568000e+01 7.0636000e-02 5.0886000e-02 /
CHEB / 1.0560000e+00 -5.0868000e-03 -3.7370000e-03 /
CHEB / 2.5063000e-01 -6.7203000e-03 -4.9164000e-03 /
CHEB / 5.1839000e-02 -1.2895000e-03 -8.8733000e-04 /

C2H4O+C2H3(+m)=CH3+C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.647947274101575
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1273000e+00 -8.9273000e-01 -3.8300000e-01 /
CHEB / 6.4376000e+00 1.0250000e+00 4.0217000e-01 /
CHEB / 3.9675000e-01 1.7378000e-03 4.7900000e-02 /
CHEB / -5.1246000e-02 -1.1115000e-01 -4.2391000e-02 /
CHEB / -7.0026000e-02 -3.9771000e-02 -2.8632000e-02 /

C2H4O+C2H3(+m)=C2H3O-2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.9897725292553101
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.7461000e-01 -1.5615000e+00 -6.4065000e-01 /
CHEB / 9.1200000e+00 1.8971000e+00 6.9928000e-01 /
CHEB / 6.3293000e-01 -1.4253000e-01 5.8044000e-02 /
CHEB / -8.1501000e-02 -1.9161000e-01 -9.4814000e-02 /
CHEB / -6.0047000e-02 -3.3404000e-02 -3.7290000e-02 /
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C2H4O+C2H3(+m)=C4H6-13+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.439426060980487
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9188000e+00 -6.0916000e-01 -2.2606000e-01 /
CHEB / 4.9988000e+00 6.4612000e-01 2.0065000e-01 /
CHEB / 1.8361000e-01 7.5342000e-02 7.3306000e-02 /
CHEB / -5.3574000e-02 -7.2135000e-02 -1.4989000e-02 /
CHEB / -6.7268000e-02 -4.7964000e-02 -2.8680000e-02 /

C2H4O+C2H3(+m)=nC4H5+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.358567236538022
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.2892000e+00 -5.2319000e-01 -2.8623000e-01 /
CHEB / 1.5481000e+01 5.8790000e-01 3.0808000e-01 /
CHEB / 7.8799000e-01 2.8350000e-02 3.1987000e-02 /
CHEB / 1.3448000e-01 -7.8295000e-02 -3.9512000e-02 /
CHEB / 1.7260000e-02 -3.0260000e-02 -2.1614000e-02 /

C2H4O+C2H3(+m)=CH3+C3H3OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.2399917660729356
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9864000e+00 -1.0606000e+00 -3.5562000e-01 /
CHEB / 8.0485000e+00 1.2683000e+00 3.5608000e-01 /
CHEB / 5.7566000e-01 -6.6433000e-02 7.8156000e-02 /
CHEB / -1.3582000e-02 -1.3002000e-01 -5.4794000e-02 /
CHEB / -4.7884000e-02 -3.3940000e-02 -3.1824000e-02 /

C2H4O+C2H3(+m)=CH3+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.02795848433408
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8915000e-01 -5.6091000e-01 -2.0142000e-01 /
CHEB / 7.2448000e+00 6.2392000e-01 1.9012000e-01 /
CHEB / 5.6126000e-01 2.5728000e-02 5.1611000e-02 /
CHEB / 4.2199000e-02 -6.4892000e-02 -1.8491000e-02 /
CHEB / -2.9826000e-02 -3.2849000e-02 -2.1801000e-02 /

C2H4O+C2H3(+m)=CH3CHO+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.118728856467797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0226000e+00 -5.5281000e-01 -2.0696000e-01 /
CHEB / 8.0647000e+00 6.3077000e-01 2.0453000e-01 /
CHEB / 7.9132000e-01 6.2818000e-03 4.3613000e-02 /
CHEB / 1.1198000e-01 -6.7197000e-02 -2.2888000e-02 /
CHEB / -5.6347000e-03 -2.8156000e-02 -2.0580000e-02 /
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C4H6-13+OH(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -45.515243862580036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1407000e-02 3.1067000e+00 -1.4371000e+00 /
CHEB / 1.3492000e+00 3.2147000e+00 8.6006000e-01 /
CHEB / -2.4212000e+00 3.9466000e-01 3.5437000e-01 /
CHEB / -1.5575000e+00 -2.8290000e-01 2.0448000e-02 /
CHEB / -7.4945000e-01 -2.9330000e-01 -5.9656000e-02 /

C4H6-13+OH(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -45.515243862580036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8878000e-01 3.1298000e+00 -1.1903000e+00 /
CHEB / 1.5218000e+00 2.9434000e+00 5.5095000e-01 /
CHEB / -2.3996000e+00 4.8348000e-01 3.0877000e-01 /
CHEB / -1.5323000e+00 -2.1133000e-01 6.9430000e-02 /
CHEB / -7.4454000e-01 -2.7770000e-01 -2.7618000e-02 /

C4H6-13+OH(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -48.414915057819684
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7732000e+00 3.1135000e+00 -1.0615000e+00 /
CHEB / -2.5677000e-01 2.7058000e+00 5.1822000e-01 /
CHEB / -2.6765000e+00 5.2847000e-01 2.3865000e-01 /
CHEB / -1.5067000e+00 -1.7461000e-01 6.0438000e-02 /
CHEB / -7.1416000e-01 -2.4233000e-01 -2.3023000e-02 /

C4H6-13+OH(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -48.21498547488225
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1631000e+00 3.6973000e+00 -9.3827000e-01 /
CHEB / 2.6973000e-01 2.2622000e+00 3.8406000e-01 /
CHEB / -2.3714000e+00 5.0657000e-01 2.2129000e-01 /
CHEB / -1.3971000e+00 -1.5857000e-01 7.3794000e-02 /
CHEB / -7.0020000e-01 -2.4270000e-01 -1.4806000e-02 /

C4H6-13+OH(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -48.21498547488225
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5257000e+00 1.3860000e+00 -9.1573000e-01 /
CHEB / 1.0850000e+00 3.5691000e+00 3.2638000e-01 /
CHEB / -2.2481000e+00 7.1133000e-01 3.3264000e-01 /
CHEB / -1.3717000e+00 -1.5088000e-01 8.2036000e-02 /
CHEB / -6.8515000e-01 -2.1847000e-01 -3.1952000e-02 /
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C4H6-13+OH(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.20655783388506
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6017000e+00 2.9709000e+00 -1.5463000e+00 /
CHEB / 1.0789000e+00 3.7303000e+00 9.7815000e-01 /
CHEB / -2.6722000e+00 1.5309000e-01 4.1097000e-01 /
CHEB / -1.5316000e+00 -5.3291000e-01 2.9580000e-03 /
CHEB / -6.0514000e-01 -3.3902000e-01 -1.0110000e-01 /

C4H6-13+OH(+m)=cHC[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.10765654966444
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0904000e+00 2.9347000e+00 -1.2651000e+00 /
CHEB / 2.1118000e+00 3.2186000e+00 9.5490000e-01 /
CHEB / -1.6543000e+00 7.9228000e-02 3.0043000e-01 /
CHEB / -9.8474000e-01 -3.1795000e-01 2.9245000e-02 /
CHEB / -4.9985000e-01 -1.9918000e-01 -4.5974000e-02 /

C4H6-13+OH(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.41717204176085
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5758000e-01 2.7619000e+00 -1.3473000e+00 /
CHEB / 1.1261000e+00 2.9629000e+00 8.2445000e-01 /
CHEB / -2.0506000e+00 2.3828000e-01 2.7934000e-01 /
CHEB / -1.1849000e+00 -3.1796000e-01 1.5752000e-02 /
CHEB / -5.4816000e-01 -2.4133000e-01 -6.0297000e-02 /

C4H6-13+OH(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/De_Cd/H2     O_pri_rad      deltaHrxn(T=298K)
= -27.88694983391427 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1092000e+01 6.5639000e-01 -5.5132000e-02 /
CHEB / -2.8841000e+00 1.0049000e+00 -3.2428000e-02 /
CHEB / -1.9749000e+00 4.4429000e-01 5.2958000e-02 /
CHEB / -1.1913000e+00 3.7426000e-02 5.4072000e-02 /
CHEB / -6.1810000e-01 -1.1568000e-01 8.7463000e-03 /

C4H6-13+OH(+m)=CH3CH[OH]CHcH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -17.788048550085403
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6734000e+00 1.8778000e-01 -3.4944000e-01 /
CHEB / 4.0542000e+00 1.6679000e+00 1.5258000e-01 /
CHEB / -1.7964000e+00 4.8942000e-01 1.2534000e-01 /
CHEB / -1.2184000e+00 -4.8920000e-02 3.8298000e-02 /
CHEB / -6.6658000e-01 -1.6489000e-01 -1.7622000e-02 /
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C4H6-13+OH(+m)=CH3CH[OH]cCH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -19.987824030039835
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1670000e+00 6.5168000e-01 -4.7670000e-01 /
CHEB / 3.5073000e+00 1.7098000e+00 2.6297000e-01 /
CHEB / -1.8310000e+00 3.7919000e-01 1.5122000e-01 /
CHEB / -1.1018000e+00 -1.0311000e-01 1.6312000e-02 /
CHEB / -5.5357000e-01 -1.4855000e-01 -3.3777000e-02 /

C4H6-13+OH(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.927211954122075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9996000e+00 4.0102000e+00 -4.2176000e-01 /
CHEB / 2.6864000e+00 -1.8336000e-02 2.1704000e-01 /
CHEB / -2.3972000e+00 -1.2689000e-01 1.9540000e-02 /
CHEB / -1.3442000e+00 -9.4813000e-02 -1.5215000e-02 /
CHEB / -6.1559000e-01 -8.5207000e-02 6.8858000e-03 /

C4H6-13+OH(+m)=CH2CO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.98802968585537
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6650000e+00 -1.8422000e+00 -6.1070000e-01 /
CHEB / 5.9340000e+00 2.0529000e+00 5.7541000e-01 /
CHEB / -3.1967000e-02 8.8970000e-02 1.5379000e-01 /
CHEB / -3.2778000e-01 -2.2686000e-01 -4.8134000e-02 /
CHEB / -1.8939000e-01 -1.0162000e-01 -6.5485000e-02 /

C4H6-13+OH(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -26.036979972571473
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3835000e+00 -1.3500000e+00 -4.8251000e-01 /
CHEB / 5.3426000e+00 1.4612000e+00 4.6237000e-01 /
CHEB / -1.5812000e-01 1.1942000e-01 1.0619000e-01 /
CHEB / -3.3905000e-01 -1.4781000e-01 -2.6797000e-02 /
CHEB / -2.0455000e-01 -8.7292000e-02 -4.2829000e-02 /

C4H6-13+OH(+m)=C4H6O(717)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -15.938602816667718
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4971000e+00 -1.2866000e+00 -4.4132000e-01 /
CHEB / 4.8114000e+00 1.4059000e+00 4.2063000e-01 /
CHEB / -6.4794000e-02 9.5564000e-02 1.0051000e-01 /
CHEB / -2.1348000e-01 -1.4985000e-01 -3.0194000e-02 /
CHEB / -1.2368000e-01 -7.7507000e-02 -3.9981000e-02 /
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C4H6-13+OH(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -38.86601265615642
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0030000e+01 -2.2815000e-02 -1.7876000e-02 /
CHEB / 2.5851000e+01 3.1265000e-02 2.4594000e-02 /
CHEB / 5.1621000e-01 -6.6485000e-03 -5.3849000e-03 /
CHEB / 4.6481000e-02 -2.6688000e-03 -2.0743000e-03 /
CHEB / -2.4461000e-02 3.6766000e-04 3.6143000e-04 /

C4H6-13+OH(+m)=CH3+C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.208521213121088
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6744000e+00 -1.3235000e+00 -4.5535000e-01 /
CHEB / 4.4239000e+00 1.4720000e+00 4.4235000e-01 /
CHEB / -1.8039000e-01 6.2792000e-02 9.3530000e-02 /
CHEB / -2.6295000e-01 -1.5546000e-01 -3.3219000e-02 /
CHEB / -1.4305000e-01 -7.1754000e-02 -4.0120000e-02 /

C4H6-13+OH(+m)=nC4H5+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.919141175557534
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8521000e+00 -4.4656000e-01 -2.6750000e-01 /
CHEB / 1.5425000e+01 5.0112000e-01 2.8892000e-01 /
CHEB / 1.4584000e-01 3.1735000e-02 3.2190000e-02 /
CHEB / -8.9492000e-02 -7.0581000e-02 -3.8412000e-02 /
CHEB / -6.3357000e-02 -3.1022000e-02 -2.2633000e-02 /

C4H6-13+OH(+m)=CH3+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.58853242335359
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2730000e+00 -5.7469000e-01 -2.2771000e-01 /
CHEB / 6.1945000e+00 6.0410000e-01 2.1160000e-01 /
CHEB / -2.0538000e-01 7.1164000e-02 5.9307000e-02 /
CHEB / -1.7545000e-01 -5.8596000e-02 -1.4100000e-02 /
CHEB / -1.0217000e-01 -4.4208000e-02 -2.3825000e-02 /

C4H6-13+OH(+m)=CH3CHO+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -4.6793027954873025
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5941000e+00 -5.6927000e-01 -2.3449000e-01 /
CHEB / 7.0207000e+00 6.2412000e-01 2.2988000e-01 /
CHEB / 6.2605000e-02 4.4083000e-02 5.0793000e-02 /
CHEB / -9.2351000e-02 -6.8934000e-02 -2.1684000e-02 /
CHEB / -7.4721000e-02 -3.9234000e-02 -2.3964000e-02 /
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C2H5O-2+C2H2(+m)=cH2C[O]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.05453486078831
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8136000e+00 4.9721000e+00 -1.4969000e+00 /
CHEB / 2.0528000e+00 2.9844000e+00 1.0446000e+00 /
CHEB / -2.4205000e+00 1.1073000e-01 4.4029000e-01 /
CHEB / -1.5431000e+00 -3.6504000e-01 8.4660000e-03 /
CHEB / -7.7867000e-01 -2.8238000e-01 -6.8188000e-02 /

C2H5O-2+C2H2(+m)=CH3C[O]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.05453486078831
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2774000e+00 4.7814000e+00 -1.2403000e+00 /
CHEB / 2.3931000e+00 2.8883000e+00 6.9993000e-01 /
CHEB / -2.3612000e+00 2.5564000e-01 4.1082000e-01 /
CHEB / -1.5258000e+00 -2.9375000e-01 7.2560000e-02 /
CHEB / -7.8863000e-01 -2.8669000e-01 -3.8407000e-02 /

C2H5O-2+C2H2(+m)=CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.95420605602796
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.3905000e+00 4.7566000e+00 -8.8259000e-01 /
CHEB / 7.5323000e-01 2.5853000e+00 4.4271000e-01 /
CHEB / -2.6082000e+00 3.4319000e-01 2.8175000e-01 /
CHEB / -1.5008000e+00 -2.3193000e-01 1.0181000e-01 /
CHEB / -7.6084000e-01 -2.4244000e-01 -1.0699000e-02 /

C2H5O-2+C2H2(+m)=CH3C[OH]CHcH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.75427647309052
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0431000e+00 5.2490000e+00 -8.0852000e-01 /
CHEB / 1.3156000e+00 2.2367000e+00 3.6747000e-01 /
CHEB / -2.3195000e+00 2.9535000e-01 2.5994000e-01 /
CHEB / -1.4040000e+00 -2.3444000e-01 1.0644000e-01 /
CHEB / -7.4880000e-01 -2.4474000e-01 -4.0868000e-03 /

C2H5O-2+C2H2(+m)=CH2C[OH]cHCH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -53.75427647309052
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2410000e+00 3.1997000e+00 -1.1044000e+00 /
CHEB / 1.7409000e+00 3.3563000e+00 6.5947000e-01 /
CHEB / -2.2543000e+00 4.2248000e-01 3.8569000e-01 /
CHEB / -1.3563000e+00 -2.0508000e-01 7.2816000e-02 /
CHEB / -7.2033000e-01 -1.9161000e-01 -3.2815000e-02 /
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```
C2H5O-2+C2H2(+m)=CH2C[OH]CH2cH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.74584883209333
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2363000e+00 5.0306000e+00 -1.5947000e+00 /
CHEB / 1.6292000e+00 3.2964000e+00 1.1607000e+00 /
CHEB / -2.6833000e+00 -1.5757000e-01 4.7743000e-01 /
CHEB / -1.5034000e+00 -5.9318000e-01 7.5412000e-03 /
CHEB / -6.2894000e-01 -3.2119000e-01 -9.7051000e-02 /

C2H5O-2+C2H2(+m)=cHC[OH]C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.646947547872713
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7859000e+00 4.8780000e+00 -1.2430000e+00 /
CHEB / 2.7379000e+00 2.7635000e+00 1.1137000e+00 /
CHEB / -1.6225000e+00 -1.7665000e-01 3.9987000e-01 /
CHEB / -9.6794000e-01 -3.7422000e-01 2.4212000e-02 /
CHEB / -5.3413000e-01 -1.9132000e-01 -5.9018000e-02 /

C2H5O-2+C2H2(+m)=CH3C[OH]cCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -32.95646303996912
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8579000e+00 4.7035000e+00 -1.1870000e+00 /
CHEB / 2.0012000e+00 2.5679000e+00 7.9141000e-01 /
CHEB / -1.9832000e+00 1.4378000e-02 2.7786000e-01 /
CHEB / -1.1632000e+00 -3.7836000e-01 5.0176000e-02 /
CHEB / -5.9088000e-01 -2.3406000e-01 -4.0855000e-02 /

C2H5O-2+C2H2(+m)=cH2CH[OH]C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -33.426240832122545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9993000e-01 1.8948000e+00 -8.3135000e-01 /
CHEB / 1.7681000e+00 2.2869000e+00 2.9543000e-01 /
CHEB / -2.0625000e+00 4.5274000e-01 2.2579000e-01 /
CHEB / -1.3587000e+00 -1.5252000e-01 5.9813000e-02 /
CHEB / -7.2204000e-01 -2.1425000e-01 -2.5346000e-02 /

C2H5O-2+C2H2(+m)=CH3CH[OH]CHcH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_rad/H/CsO     Ct/H_Ct/H        deltaHrxn(T=298K)
= -23.327339548293676 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1238000e+00 6.0047000e-01 -6.0223000e-02 /
CHEB / -2.3386000e-01 9.2064000e-01 -4.2484000e-02 /
CHEB / -1.9080000e+00 4.2202000e-01 4.1530000e-02 /
CHEB / -1.1859000e+00 5.0444000e-02 5.0550000e-02 /
CHEB / -6.5426000e-01 -1.0372000e-01 1.4128000e-02 /
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C2H5O-2+C2H2(+m)=CH3CH[OH]cCH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -25.527115028248108
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8051000e-01 1.4206000e+00 -3.1440000e-01 /
CHEB / 3.1739000e+00 2.4266000e+00 -1.0850000e-02 /
CHEB / -1.8251000e+00 4.0270000e-02 2.2048000e-01 /
CHEB / -1.1823000e+00 -1.3425000e-01 4.7262000e-02 /
CHEB / -6.0607000e-01 -1.4934000e-01 -2.9454000e-02 /

C2H5O-2+C2H2(+m)=CH3CH[o]C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.466502952330348
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3677000e-01 2.7092000e+00 -5.2471000e-01 /
CHEB / -2.8524000e-01 7.2640000e-01 2.1362000e-01 /
CHEB / -2.3671000e+00 1.2856000e-01 7.7720000e-02 /
CHEB / -1.4278000e+00 -1.2058000e-01 4.1545000e-02 /
CHEB / -6.9652000e-01 -1.4896000e-01 2.4205000e-03 /

C2H5O-2+C2H2(+m)=CH2CO+C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.527320684063643
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3635000e-01 -1.5960000e+00 -4.6130000e-01 /
CHEB / 6.9812000e+00 1.7102000e+00 4.2252000e-01 /
CHEB / -7.1647000e-02 1.4514000e-01 1.2034000e-01 /
CHEB / -3.3028000e-01 -1.6882000e-01 -2.7190000e-02 /
CHEB / -1.7407000e-01 -9.4224000e-02 -4.0047000e-02 /

C2H5O-2+C2H2(+m)=CH3CO+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.576270970779746
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0883000e+00 -1.1997000e+00 -2.7250000e-01 /
CHEB / 6.7440000e+00 1.1968000e+00 2.1923000e-01 /
CHEB / -1.2320000e-01 2.0273000e-01 9.1089000e-02 /
CHEB / -3.5114000e-01 -8.7973000e-02 1.2792000e-02 /
CHEB / -2.0988000e-01 -8.9546000e-02 -2.3536000e-02 /

C2H5O-2+C2H2(+m)=C4H6O(717)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.477893814876005
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3009000e+00 -1.2064000e+00 -1.2646000e-01 /
CHEB / 4.8413000e+00 1.1741000e+00 3.9819000e-02 /
CHEB / 3.4101000e-01 2.6230000e-01 9.1542000e-02 /
CHEB / -1.7533000e-01 -1.0824000e-01 5.3903000e-02 /
CHEB / -1.6833000e-01 -1.1831000e-01 -2.2330000e-02 /
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C2H5O-2+C2H2(+m)=C3H7-1+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -44.405303654364694
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1023000e+01 -3.8337000e-02 -3.0135000e-02 /
CHEB / 2.4192000e+01 4.8653000e-02 3.8175000e-02 /
CHEB / 6.9037000e-01 -5.0540000e-03 -3.7315000e-03 /
CHEB / 1.4798000e-01 -6.7615000e-03 -5.5231000e-03 /
CHEB / 2.6910000e-02 -4.8890000e-05 -7.5004000e-05 /

C2H5O-2+C2H2(+m)=CH3+C3H4O-enone(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (cH2C[O]C2H5)   deltaHrxn(T=298K) = -
21.74781221132936 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6943000e+00 -1.2061000e+00 -2.8311000e-01 /
CHEB / 5.6801000e+00 1.2394000e+00 2.3175000e-01 /
CHEB / -1.7782000e-01 1.6717000e-01 9.1425000e-02 /
CHEB / -2.7504000e-01 -1.0518000e-01 9.6461000e-03 /
CHEB / -1.3957000e-01 -8.6210000e-02 -2.6165000e-02 /

C2H5O-2+C2H2(+m)=C2H3O-2+C2H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -1.0896374664830955
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.9994000e-01 -1.8016000e+00 -5.8316000e-01 /
CHEB / 8.0871000e+00 2.0697000e+00 5.8584000e-01 /
CHEB / 7.8910000e-02 -1.6264000e-02 9.9014000e-02 /
CHEB / -2.6891000e-01 -1.9935000e-01 -5.5721000e-02 /
CHEB / -1.1417000e-01 -7.0653000e-02 -4.0989000e-02 /

C2H5O-2+C2H2(+m)=C2H4O+C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -0.09986493722779244
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0829000e-01 -1.4071000e+00 -3.4154000e-01 /
CHEB / 8.1439000e+00 1.5358000e+00 2.7393000e-01 /
CHEB / 4.0867000e-01 1.0195000e-01 1.4258000e-01 /
CHEB / -1.4529000e-01 -1.5813000e-01 -1.7192000e-02 /
CHEB / -1.0267000e-01 -8.6615000e-02 -4.6198000e-02 /

C2H5O-2+C2H2(+m)=C4H6-13+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.539290998208273
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5792000e+00 -1.5653000e+00 -3.2620000e-01 /
CHEB / 5.5408000e+00 1.5962000e+00 2.3743000e-01 /
CHEB / -1.6129000e-01 2.3140000e-01 1.4623000e-01 /
CHEB / -3.5335000e-01 -1.3677000e-01 8.8337000e-03 /
CHEB / -1.9457000e-01 -1.1258000e-01 -3.8661000e-02 /
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```
C2H5O-2+C2H2(+m)=nC4H5+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.458432173765807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7420000e+00 -2.8621000e-01 -1.6671000e-01 /
CHEB / 1.2448000e+01 3.0763000e-01 1.7024000e-01 /
CHEB / 4.3900000e-02 4.0013000e-02 3.2708000e-02 /
CHEB / -4.5190000e-02 -4.5805000e-02 -2.2164000e-02 /
CHEB / -2.4805000e-02 -2.6095000e-02 -1.8072000e-02 /

C2H5O-2+C2H2(+m)=CH3+C3H3OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.339856703300721
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1606000e+00 -1.0979000e+00 -3.4340000e-01 /
CHEB / 7.2550000e+00 1.1932000e+00 3.1432000e-01 /
CHEB / -1.6299000e-01 7.7459000e-02 9.6067000e-02 /
CHEB / -2.5419000e-01 -1.0658000e-01 -2.8339000e-02 /
CHEB / -1.1956000e-01 -7.2550000e-02 -2.6564000e-02 /

C2H5O-2+C2H2(+m)=CH3+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.127823421561864
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0262000e+00 -1.2619000e+00 -1.1385000e-01 /
CHEB / 3.1267000e+00 1.1257000e+00 3.5495000e-02 /
CHEB / -3.5231000e-01 3.2627000e-01 6.6286000e-02 /
CHEB / -3.2671000e-01 -2.7144000e-02 5.3599000e-02 /
CHEB / -1.5305000e-01 -1.0231000e-01 -4.2772000e-04 /

C2H5O-2+C2H2(+m)=CH3CHO+C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.218593793695575
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2127000e+00 -1.2318000e+00 -1.2707000e-01 /
CHEB / 4.0396000e+00 1.1608000e+00 4.9071000e-02 /
CHEB / -8.8831000e-02 2.7381000e-01 7.7267000e-02 /
CHEB / -2.2115000e-01 -6.1728000e-02 4.8334000e-02 /
CHEB / -1.0053000e-01 -1.0434000e-01 -9.7467000e-03 /

nC4H5+H2O(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.5961026870225
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6108000e+01 1.0314000e+01 -2.1091000e+00 /
CHEB / 1.4706000e+01 1.5261000e+00 1.5534000e+00 /
CHEB / -2.4041000e+00 -3.4210000e-01 5.6114000e-01 /
CHEB / -1.4782000e+00 -4.1519000e-01 7.5392000e-02 /
CHEB / -7.5162000e-01 -2.5667000e-01 -3.9561000e-02 /
```

```
nC4H5+H2O(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.5961026870225
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6737000e+01 9.8660000e+00 -1.9506000e+00 /
CHEB / 1.5232000e+01 1.7115000e+00 1.2968000e+00 /
CHEB / -2.3366000e+00 -1.7427000e-01 5.6551000e-01 /
CHEB / -1.4881000e+00 -3.8634000e-01 1.2445000e-01 /
CHEB / -7.6963000e-01 -2.7661000e-01 -2.4214000e-02 /

nC4H5+H2O(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.49577388226215
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4982000e+01 9.7586000e+00 -1.4505000e+00 /
CHEB / 1.3733000e+01 1.4602000e+00 8.1935000e-01 /
CHEB / -2.5833000e+00 -3.9229000e-02 5.0328000e-01 /
CHEB / -1.4692000e+00 -3.2356000e-01 1.7206000e-01 /
CHEB / -7.4826000e-01 -2.4371000e-01 -1.2731000e-03 /

nC4H5+H2O(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.29584429932471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4643000e+01 1.0235000e+01 -1.3912000e+00 /
CHEB / 1.4301000e+01 1.1288000e+00 7.5965000e-01 /
CHEB / -2.2993000e+00 -9.3190000e-02 4.7664000e-01 /
CHEB / -1.3736000e+00 -3.2795000e-01 1.7294000e-01 /
CHEB / -7.3680000e-01 -2.4558000e-01 5.3557000e-03 /

nC4H5+H2O(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -37.29584429932471
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3528000e+01 8.5361000e+00 -1.7254000e+00 /
CHEB / 1.4367000e+01 1.8413000e+00 1.1758000e+00 /
CHEB / -2.2025000e+00 5.2220000e-03 5.2390000e-01 /
CHEB / -1.2834000e+00 -2.5356000e-01 1.5355000e-01 /
CHEB / -6.9718000e-01 -1.8063000e-01 -2.1425000e-03 /

nC4H5+H2O(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.28741665832752
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7378000e+01 1.0613000e+01 -2.1022000e+00 /
CHEB / 1.4093000e+01 1.5377000e+00 1.5491000e+00 /
CHEB / -2.6411000e+00 -5.7347000e-01 6.0083000e-01 /
CHEB / -1.4240000e+00 -6.1411000e-01 8.9196000e-02 /
CHEB / -6.0483000e-01 -2.9361000e-01 -7.0266000e-02 /
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nC4H5+H2O(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.188515374106908
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8891000e+01 1.0118000e+01 -1.5891000e+00 /
CHEB / 1.5391000e+01 9.2393000e-01 1.6760000e+00 /
CHEB / -1.6295000e+00 -4.4834000e-01 4.4674000e-01 /
CHEB / -9.6396000e-01 -2.9881000e-01 -8.8360000e-04 /
CHEB / -5.0935000e-01 -1.8006000e-01 -3.4207000e-02 /

nC4H5+H2O(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.498030866203315
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7265000e+01 9.9804000e+00 -1.6333000e+00 /
CHEB / 1.4782000e+01 1.0824000e+00 1.0764000e+00 /
CHEB / -1.9287000e+00 -3.7730000e-01 4.7711000e-01 /
CHEB / -1.1077000e+00 -4.5168000e-01 1.5210000e-01 /
CHEB / -5.6662000e-01 -2.3249000e-01 -1.9531000e-02 /

nC4H5+H2O(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -16.967808658356734
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0267000e+01 7.2881000e+00 -1.6550000e+00 /
CHEB / 1.4998000e+01 9.3646000e-01 9.3710000e-01 /
CHEB / -2.2245000e+00 6.7103000e-02 3.7993000e-01 /
CHEB / -1.3508000e+00 -2.1313000e-01 8.0482000e-02 /
CHEB / -7.0674000e-01 -1.8147000e-01 -2.6935000e-02 /

nC4H5+H2O(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: 1,3_Insertion_ROR estimate:
(Average:) Cd/H2_Cd/H/De     H_OH         deltaHrxn(T=298K) = -
6.868907374527868 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6106000e+01 5.0005000e+00 -1.0565000e+00 /
CHEB / 1.4559000e+01 6.6307000e-01 5.7912000e-01 /
CHEB / -2.2364000e+00 1.9171000e-01 2.7334000e-01 /
CHEB / -1.3082000e+00 -8.8347000e-02 6.2105000e-02 /
CHEB / -6.8524000e-01 -1.2029000e-01 -2.7250000e-02 /

nC4H5+H2O(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.0686828544823
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0734000e+01 6.5397000e+00 -1.0478000e+00 /
CHEB / 1.5570000e+01 4.6153000e-01 7.9999000e-01 /
CHEB / -1.8090000e+00 -7.8924000e-02 3.5676000e-01 /
CHEB / -1.1070000e+00 -1.9897000e-01 7.3383000e-02 /
CHEB / -6.0429000e-01 -1.1776000e-01 -4.0412000e-02 /
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nC4H5+H2O(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -14.00807077856454
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3038000e+01 7.3198000e+00 -1.4050000e+00 /
CHEB / 1.4336000e+01 1.8666000e-01 6.8448000e-01 /
CHEB / -2.6625000e+00 -5.1564000e-02 3.3229000e-01 /
CHEB / -1.5315000e+00 -2.2891000e-01 7.1537000e-02 /
CHEB / -7.3077000e-01 -1.7059000e-01 -3.9605000e-02 /

nC4H5+H2O(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -8.068888510297828
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4978000e+01 -4.8768000e-01 -3.0083000e-01 /
CHEB / 2.0162000e+01 5.7020000e-01 3.4384000e-01 /
CHEB / 3.4125000e-01 -2.6938000e-03 8.1567000e-03 /
CHEB / -2.6620000e-02 -7.1624000e-02 -4.2998000e-02 /
CHEB / -3.8394000e-02 -2.2329000e-02 -1.5730000e-02 /

nC4H5+H2O(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -15.11783879701394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5260000e+01 -2.8977000e-01 -1.7763000e-01 /
CHEB / 2.0301000e+01 3.2656000e-01 1.9352000e-01 /
CHEB / 3.3094000e-01 2.6169000e-02 2.2949000e-02 /
CHEB / -5.4327000e-02 -5.0963000e-02 -2.7372000e-02 /
CHEB / -6.4544000e-02 -2.4395000e-02 -1.7249000e-02 /

nC4H5+H2O(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.01946164111019
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3650000e+01 -3.1855000e-01 -1.8407000e-01 /
CHEB / 1.9604000e+01 3.4446000e-01 1.9188000e-01 /
CHEB / 4.1243000e-01 3.9394000e-02 2.9841000e-02 /
CHEB / 5.0631000e-02 -4.9924000e-02 -2.4571000e-02 /
CHEB / -2.4668000e-04 -2.5906000e-02 -1.7270000e-02 /

nC4H5+H2O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.946871480598887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1310000e+01 -1.0299000e-01 -7.0841000e-02 /
CHEB / 3.2187000e+01 1.2000000e-01 8.2209000e-02 /
CHEB / 1.4698000e+00 -1.2441000e-03 -3.4312000e-04 /
CHEB / 4.2473000e-01 -1.5183000e-02 -1.0509000e-02 /
CHEB / 1.2559000e-01 -3.4682000e-03 -2.5341000e-03 /
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nC4H5+H2O(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.289380037563554
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3220000e+01 -3.4778000e-01 -1.9886000e-01 /
CHEB / 1.9104000e+01 3.8014000e-01 2.0987000e-01 /
CHEB / 2.5706000e-01 3.4555000e-02 2.7185000e-02 /
CHEB / 6.5736000e-03 -5.1641000e-02 -2.5118000e-02 /
CHEB / -1.3077000e-02 -2.5839000e-02 -1.7287000e-02 /

nC4H5+H2O(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.669391247796055
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3577000e+01 -2.5447000e-01 -1.6112000e-01 /
CHEB / 1.8165000e+01 2.7809000e-01 1.6648000e-01 /
CHEB / 6.2533000e-02 3.4850000e-02 3.1627000e-02 /
CHEB / 1.7036000e-03 -4.4903000e-02 -2.3102000e-02 /
CHEB / 1.1802000e-02 -2.5500000e-02 -1.8670000e-02 /

CH3+C3H3OH(+m)=cH2C[O]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -47.71467815748759
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5383000e+00 5.0565000e+00 -1.5699000e+00 /
CHEB / 2.8542000e+00 2.9087000e+00 1.0861000e+00 /
CHEB / -2.3880000e+00 7.9316000e-02 4.3036000e-01 /
CHEB / -1.4395000e+00 -3.5923000e-01 -3.9957000e-03 /
CHEB / -6.8660000e-01 -2.6042000e-01 -7.5770000e-02 /

CH3+C3H3OH(+m)=CH3C[O]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -47.71467815748759
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.9777000e+00 4.8994000e+00 -1.3065000e+00 /
CHEB / 3.1814000e+00 2.7966000e+00 7.4240000e-01 /
CHEB / -2.3401000e+00 2.0689000e-01 3.9511000e-01 /
CHEB / -1.4253000e+00 -2.9351000e-01 5.5859000e-02 /
CHEB / -6.9347000e-01 -2.6045000e-01 -4.5479000e-02 /

CH3+C3H3OH(+m)=CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.61434935272724
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0585000e+00 4.8859000e+00 -9.9428000e-01 /
CHEB / 1.5239000e+00 2.5024000e+00 5.3272000e-01 /
CHEB / -2.5964000e+00 2.8713000e-01 2.7489000e-01 /
CHEB / -1.4034000e+00 -2.4170000e-01 7.6614000e-02 /
CHEB / -6.6662000e-01 -2.1974000e-01 -2.2086000e-02 /
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CH3+C3H3OH(+m)=CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.4144197697898
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.7069000e+00 5.3860000e+00 -9.1578000e-01 /
CHEB / 2.0871000e+00 2.1525000e+00 4.5333000e-01 /
CHEB / -2.3037000e+00 2.4392000e-01 2.5328000e-01 /
CHEB / -1.3044000e+00 -2.4122000e-01 8.2145000e-02 /
CHEB / -6.5369000e-01 -2.2074000e-01 -1.4894000e-02 /

CH3+C3H3OH(+m)=CH2C[OH]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -50.4144197697898
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9659000e+00 3.2897000e+00 -1.1694000e+00 /
CHEB / 2.5491000e+00 3.2906000e+00 6.9685000e-01 /
CHEB / -2.2232000e+00 3.8851000e-01 3.7618000e-01 /
CHEB / -1.2550000e+00 -2.0692000e-01 5.6968000e-02 /
CHEB / -6.2713000e-01 -1.7262000e-01 -4.2182000e-02 /

CH3+C3H3OH(+m)=CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.405992128792604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9846000e+00 5.0831000e+00 -1.6749000e+00 /
CHEB / 2.4457000e+00 3.2447000e+00 1.2064000e+00 /
CHEB / -2.6449000e+00 -1.7856000e-01 4.7276000e-01 /
CHEB / -1.3991000e+00 -5.8713000e-01 -5.1911000e-03 /
CHEB / -5.3801000e-01 -3.0199000e-01 -1.0710000e-01 /

CH3+C3H3OH(+m)=cHC[OH]C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -24.307090844571995
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5246000e+00 4.9574000e+00 -1.3300000e+00 /
CHEB / 3.5441000e+00 2.7177000e+00 1.1555000e+00 /
CHEB / -1.5917000e+00 -2.1200000e-01 3.9145000e-01 /
CHEB / -8.6194000e-01 -3.7670000e-01 1.5177000e-02 /
CHEB / -4.4019000e-01 -1.7241000e-01 -6.4434000e-02 /

CH3+C3H3OH(+m)=CH3C[OH]cCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -29.616606336668404
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5519000e+00 4.7937000e+00 -1.3006000e+00 /
CHEB / 2.7861000e+00 2.5037000e+00 8.7587000e-01 /
CHEB / -1.9694000e+00 -2.9305000e-02 2.8431000e-01 /
CHEB / -1.0647000e+00 -3.8162000e-01 3.0012000e-02 /
CHEB / -4.9694000e-01 -2.1198000e-01 -5.4286000e-02 /
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```
CH3+C3H3OH(+m)=cH2CH[OH]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -30.086384128821823
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2059000e+00 2.0494000e+00 -8.7190000e-01 /
CHEB / 2.5060000e+00 2.1981000e+00 3.6551000e-01 /
CHEB / -2.1084000e+00 3.5603000e-01 2.1971000e-01 /
CHEB / -1.2705000e+00 -1.8058000e-01 3.6481000e-02 /
CHEB / -6.2929000e-01 -1.9429000e-01 -3.3587000e-02 /

CH3+C3H3OH(+m)=CH3CH[OH]CHcH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -19.987482844992957
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.2191000e-01 9.5932000e-01 -3.9708000e-01 /
CHEB / 4.7994000e+00 2.1289000e+00 -2.0790000e-02 /
CHEB / -1.8708000e+00 1.2654000e-01 2.5754000e-01 /
CHEB / -1.3024000e+00 -2.3660000e-02 3.0671000e-02 /
CHEB / -6.5867000e-01 -1.4121000e-01 -3.2945000e-02 /

CH3+C3H3OH(+m)=CH3CH[OH]cCH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_methyl     Cd/H/Nd_Ca          deltaHrxn(T=298K)
= -22.18725832494739 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2921000e+00 7.6508000e-01 -7.7772000e-02 /
CHEB / 3.6873000e-01 9.9387000e-01 7.7662000e-04 /
CHEB / -1.9436000e+00 3.3516000e-01 6.4356000e-02 /
CHEB / -1.0827000e+00 -1.6972000e-02 3.2508000e-02 /
CHEB / -5.4286000e-01 -9.8061000e-02 -6.9183000e-03 /

CH3+C3H3OH(+m)=CH3CH[o]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.12664624902963
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7546000e+00 2.8508000e+00 -5.5019000e-01 /
CHEB / 2.0122000e-01 8.9889000e-01 2.8543000e-01 /
CHEB / -2.4886000e+00 3.5788000e-02 1.0144000e-01 /
CHEB / -1.3605000e+00 -1.9300000e-01 2.1375000e-02 /
CHEB / -5.9006000e-01 -1.4117000e-01 -1.9158000e-02 /

CH3+C3H3OH(+m)=CH2CO+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.187463980762917
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0032000e-01 -1.2999000e+00 -5.1682000e-01 /
CHEB / 7.8070000e+00 1.5151000e+00 5.3494000e-01 /
CHEB / 1.1049000e-01 -1.5805000e-02 8.4483000e-02 /
CHEB / -1.5679000e-01 -1.7917000e-01 -6.9370000e-02 /
CHEB / -9.7218000e-02 -5.0842000e-02 -4.3180000e-02 /
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CH3+C3H3OH(+m)=CH3CO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.236414267479027
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1222000e+00 -8.7377000e-01 -3.3809000e-01 /
CHEB / 7.5241000e+00 1.0029000e+00 3.4898000e-01 /
CHEB / 2.1734000e-02 1.7192000e-02 5.6119000e-02 /
CHEB / -1.8339000e-01 -1.1862000e-01 -3.7634000e-02 /
CHEB / -1.1993000e-01 -4.5411000e-02 -3.0604000e-02 /

CH3+C3H3OH(+m)=C4H6O(717)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.13803711157528
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8876000e+00 -9.6323000e-01 -1.8216000e-01 /
CHEB / 6.1591000e+00 1.1288000e+00 1.2752000e-01 /
CHEB / 4.6593000e-01 -9.4154000e-03 1.1122000e-01 /
CHEB / -9.8053000e-02 -1.5407000e-01 -1.4986000e-02 /
CHEB / -7.6181000e-02 -2.6455000e-02 -4.8291000e-02 /

CH3+C3H3OH(+m)=C3H7-1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -41.065446951063976
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1783000e+01 -2.3801000e-02 -1.6897000e-02 /
CHEB / 2.5848000e+01 2.6268000e-02 1.8654000e-02 /
CHEB / 8.7997000e-01 9.9511000e-04 7.2083000e-04 /
CHEB / 2.0565000e-01 -2.4369000e-03 -1.7540000e-03 /
CHEB / 3.1755000e-02 -1.3444000e-03 -9.6312000e-04 /

CH3+C3H3OH(+m)=CH3+C3H4O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.407955508028643
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6828000e+00 -8.8351000e-01 -3.3946000e-01 /
CHEB / 6.4850000e+00 1.0285000e+00 3.5553000e-01 /
CHEB / -7.5850000e-03 -1.2575000e-02 4.4963000e-02 /
CHEB / -1.0179000e-01 -1.1767000e-01 -3.9294000e-02 /
CHEB / -5.9118000e-02 -3.3695000e-02 -2.5829000e-02 /

CH3+C3H3OH(+m)=C4H6-13+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.1994342949075545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0592000e+00 -1.2606000e+00 -3.7388000e-01 /
CHEB / 6.2997000e+00 1.4233000e+00 3.4069000e-01 /
CHEB / -8.6015000e-02 4.2110000e-02 1.1595000e-01 /
CHEB / -2.1433000e-01 -1.6164000e-01 -3.6882000e-02 /
CHEB / -1.1887000e-01 -6.4795000e-02 -4.4127000e-02 /
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CH3+C3H3OH(+m)=nC4H5+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.118575470465089
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.5126000e+00 -3.7152000e-01 -2.0398000e-01 /
CHEB / 1.5043000e+01 4.1539000e-01 2.2022000e-01 /
CHEB / 4.0932000e-01 2.4160000e-02 2.1630000e-02 /
CHEB / 4.8870000e-02 -5.6354000e-02 -2.7187000e-02 /
CHEB / -1.7809000e-03 -2.2950000e-02 -1.5400000e-02 /

CH3+C3H3OH(+m)=CH3+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.787966718261146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2343000e+00 -1.0349000e+00 -1.4985000e-01 /
CHEB / 4.0733000e+00 1.1148000e+00 1.0911000e-01 /
CHEB / -6.9965000e-02 9.9458000e-02 6.7806000e-02 /
CHEB / -2.9650000e-03 -1.1954000e-01 6.7807000e-03 /
CHEB / 6.2283000e-02 -7.2177000e-02 -2.2367000e-02 /

CH3+C3H3OH(+m)=CH3CHO+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.878737090394864
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3859000e+00 -9.8315000e-01 -1.6182000e-01 /
CHEB / 5.0546000e+00 1.1130000e+00 1.2856000e-01 /
CHEB / 2.4247000e-01 3.3980000e-02 6.8724000e-02 /
CHEB / 1.1114000e-01 -1.3118000e-01 -4.7214000e-03 /
CHEB / 9.2480000e-02 -5.6375000e-02 -2.6515000e-02 /

CH3+C3H4O(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.926711439226445
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8463000e+00 3.7732000e+00 -1.4093000e+00 /
CHEB / 5.9350000e+00 2.5146000e+00 8.7428000e-01 /
CHEB / -2.6010000e+00 2.8150000e-01 3.1499000e-01 /
CHEB / -1.5260000e+00 -2.0135000e-01 2.9283000e-02 /
CHEB / -7.2247000e-01 -2.2474000e-01 -3.5115000e-02 /

CH3+C3H4O(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -28.926711439226445
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0096000e+01 3.8327000e+00 -1.1588000e+00 /
CHEB / 6.1118000e+00 2.2535000e+00 5.7697000e-01 /
CHEB / -2.6150000e+00 3.2163000e-01 2.5992000e-01 /
CHEB / -1.5143000e+00 -1.5369000e-01 6.3059000e-02 /
CHEB / -7.0999000e-01 -2.0120000e-01 -6.5598000e-03 /
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CH3+C3H4O(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.826382634466093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0250000e+00 3.8260000e+00 -1.0373000e+00 /
CHEB / 4.3396000e+00 2.0209000e+00 5.4475000e-01 /
CHEB / -2.9043000e+00 3.5825000e-01 1.9880000e-01 /
CHEB / -1.4975000e+00 -1.2870000e-01 5.3583000e-02 /
CHEB / -6.8053000e-01 -1.7079000e-01 -7.8255000e-03 /

CH3+C3H4O(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.626453051528657
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.6314000e+00 4.4147000e+00 -9.1247000e-01 /
CHEB / 4.8670000e+00 1.5793000e+00 4.1194000e-01 /
CHEB / -2.6057000e+00 3.2451000e-01 1.7369000e-01 /
CHEB / -1.3884000e+00 -1.1442000e-01 6.4310000e-02 /
CHEB / -6.6470000e-01 -1.6814000e-01 1.9588000e-03 /

CH3+C3H4O(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -31.626453051528657
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3144000e+00 2.0560000e+00 -8.6772000e-01 /
CHEB / 5.6764000e+00 2.8717000e+00 3.3303000e-01 /
CHEB / -2.4255000e+00 5.9242000e-01 2.7436000e-01 /
CHEB / -1.3436000e+00 -7.3663000e-02 9.0037000e-02 /
CHEB / -6.6111000e-01 -1.5353000e-01 -6.2966000e-03 /

CH3+C3H4O(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -15.618025410531462
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1467000e+01 3.5964000e+00 -1.5233000e+00 /
CHEB / 5.6682000e+00 3.0325000e+00 9.8553000e-01 /
CHEB / -2.8162000e+00 9.2238000e-02 3.8597000e-01 /
CHEB / -1.4946000e+00 -4.4123000e-01 1.9534000e-02 /
CHEB / -5.8922000e-01 -2.8693000e-01 -8.1982000e-02 /

CH3+C3H4O(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -5.519124126310851
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2936000e+01 3.5854000e+00 -1.2426000e+00 /
CHEB / 6.7030000e+00 2.5274000e+00 9.6993000e-01 /
CHEB / -1.8246000e+00 -1.6662000e-02 2.6988000e-01 /
CHEB / -9.5717000e-01 -2.4166000e-01 3.4735000e-02 /
CHEB / -4.7612000e-01 -1.3531000e-01 -2.6153000e-02 /
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CH3+C3H4O(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -10.82863961840726
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0683000e+01 3.4403000e+00 -1.3285000e+00 /
CHEB / 5.7191000e+00 2.2669000e+00 8.4175000e-01 /
CHEB / -2.2470000e+00 1.1449000e-01 2.5467000e-01 /
CHEB / -1.1644000e+00 -2.5137000e-01 2.2494000e-02 /
CHEB / -5.1975000e-01 -1.7598000e-01 -4.4964000e-02 /

CH3+C3H4O(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.298417410560678
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3193000e+00 3.0172000e+00 -7.7727000e-01 /
CHEB / 8.0487000e+00 1.3138000e+00 3.1596000e-01 /
CHEB / -2.2787000e+00 2.4627000e-01 2.0383000e-01 /
CHEB / -1.2657000e+00 -1.0129000e-01 5.2691000e-02 /
CHEB / -6.3410000e-01 -1.5337000e-01 -1.8854000e-02 /

CH3+C3H4O(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.399291606686244
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0353000e+00 4.0928000e-01 -1.3522000e-01 /
CHEB / 6.3873000e+00 1.0391000e+00 1.4363000e-01 /
CHEB / -1.9211000e+00 2.9774000e-01 4.7696000e-02 /
CHEB / -1.0951000e+00 -1.6464000e-02 1.7052000e-02 /
CHEB / -5.4415000e-01 -8.0264000e-02 -1.4643000e-03 /

CH3+C3H4O(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_methyl     CO/H/De_O           deltaHrxn(T=298K)
= -8.338679530768484 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4788000e+00 7.3050000e-01 -1.0822000e-01 /
CHEB / -2.2298000e-01 7.9027000e-01 -1.2234000e-02 /
CHEB / -2.6255000e+00 1.0359000e-01 5.4985000e-02 /
CHEB / -1.3549000e+00 -1.6114000e-01 1.8256000e-02 /
CHEB / -5.5829000e-01 -1.2902000e-01 -1.2118000e-02 /

CH3+C3H4O(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -2.399497262501775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1235000e+00 -1.2319000e+00 -5.3485000e-01 /
CHEB / 1.0750000e+01 1.3834000e+00 5.5446000e-01 /
CHEB / 1.1590000e-01 4.1659000e-02 6.9558000e-02 /
CHEB / -5.3645000e-02 -1.4443000e-01 -4.6828000e-02 /
CHEB / -3.1298000e-02 -6.8123000e-02 -4.2145000e-02 /
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```
CH3+C3H4O(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -9.448447549217883
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.3609000e+00 -6.7434000e-01 -4.2035000e-01 /
CHEB / 1.0118000e+01 7.8917000e-01 4.7066000e-01 /
CHEB / -1.1536000e-01 -5.1875000e-03 2.1243000e-02 /
CHEB / -9.8891000e-02 -8.9740000e-02 -5.0043000e-02 /
CHEB / -2.8210000e-02 -3.3226000e-02 -2.5098000e-02 /

CH3+C3H4O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.27748023280283
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0219000e+01 -2.0819000e-02 -1.4801000e-02 /
CHEB / 3.1712000e+01 2.1483000e-02 1.5303000e-02 /
CHEB / 8.2207000e-01 2.4980000e-03 1.7597000e-03 /
CHEB / 2.0173000e-01 -1.7741000e-03 -1.2832000e-03 /
CHEB / 3.1652000e-02 -1.5004000e-03 -1.0765000e-03 /

CH3CHO+C2H3(+m)=cH2C[O]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -40.83594106709273
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6656000e+00 4.0623000e+00 -1.3439000e+00 /
CHEB / 2.7483000e+00 2.7682000e+00 9.2639000e-01 /
CHEB / -2.3883000e+00 2.8715000e-01 3.3737000e-01 /
CHEB / -1.4814000e+00 -2.1862000e-01 3.5972000e-02 /
CHEB / -7.0819000e-01 -2.3089000e-01 -3.9414000e-02 /

CH3CHO+C2H3(+m)=CH3C[O]CH2cH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -40.83594106709273
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.9471000e+00 4.0813000e+00 -1.0989000e+00 /
CHEB / 2.9342000e+00 2.5161000e+00 6.2713000e-01 /
CHEB / -2.3825000e+00 3.5121000e-01 2.8232000e-01 /
CHEB / -1.4627000e+00 -1.5859000e-01 7.6326000e-02 /
CHEB / -6.9739000e-01 -2.0697000e-01 -6.1139000e-03 /

CH3CHO+C2H3(+m)=CH3C[O]cHCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -43.73561226233238
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8926000e+00 4.0669000e+00 -9.6757000e-01 /
CHEB / 1.1592000e+00 2.2699000e+00 5.9281000e-01 /
CHEB / -2.6660000e+00 3.9080000e-01 2.1064000e-01 /
CHEB / -1.4400000e+00 -1.2616000e-01 6.3705000e-02 /
CHEB / -6.6498000e-01 -1.7076000e-01 -3.6476000e-03 /
```

```
CH3CHO+C2H3(+m)=CH3C[OH]CHcH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -43.535682679394945
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5098000e+00 4.6370000e+00 -8.5120000e-01 /
CHEB / 1.6879000e+00 1.8346000e+00 4.6592000e-01 /
CHEB / -2.3687000e+00 3.5744000e-01 1.8886000e-01 /
CHEB / -1.3354000e+00 -1.1809000e-01 7.3170000e-02 /
CHEB / -6.5194000e-01 -1.7184000e-01 5.0699000e-03 /

CH3CHO+C2H3(+m)=CH2C[OH]cHCH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -43.535682679394945
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1306000e+00 2.3308000e+00 -8.3052000e-01 /
CHEB / 2.4858000e+00 3.1295000e+00 3.9964000e-01 /
CHEB / -2.2214000e+00 5.9651000e-01 3.0565000e-01 /
CHEB / -1.3012000e+00 -8.9534000e-02 9.6976000e-02 /
CHEB / -6.4623000e-01 -1.5562000e-01 -8.8809000e-03 /

CH3CHO+C2H3(+m)=CH2C[OH]CH2cH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -27.52725503839775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2540000e+00 3.9246000e+00 -1.4529000e+00 /
CHEB / 2.4710000e+00 3.2692000e+00 1.0354000e+00 /
CHEB / -2.6209000e+00 7.3766000e-02 4.0539000e-01 /
CHEB / -1.4531000e+00 -4.6381000e-01 2.5765000e-02 /
CHEB / -5.7160000e-01 -2.8927000e-01 -8.3974000e-02 /

CH3CHO+C2H3(+m)=cHC[OH]C2H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -17.428353754177138
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7374000e+00 3.8920000e+00 -1.1650000e+00 /
CHEB / 3.5058000e+00 2.7499000e+00 1.0162000e+00 /
CHEB / -1.6115000e+00 -1.8734000e-02 2.9359000e-01 /
CHEB / -9.0856000e-01 -2.5702000e-01 4.7040000e-02 /
CHEB / -4.6021000e-01 -1.4269000e-01 -2.7605000e-02 /

CH3CHO+C2H3(+m)=CH3C[OH]cCH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.737869246273547
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5178000e+00 3.7293000e+00 -1.2525000e+00 /
CHEB / 2.5356000e+00 2.5019000e+00 8.8735000e-01 /
CHEB / -2.0186000e+00 1.2241000e-01 2.5912000e-01 /
CHEB / -1.1100000e+00 -2.5843000e-01 2.7205000e-02 /
CHEB / -5.0410000e-01 -1.7720000e-01 -4.3431000e-02 /
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CH3CHO+C2H3(+m)=cH2CH[OH]C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -23.207647038426966
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6991000e+00 3.1547000e+00 -7.8615000e-01 /
CHEB / 4.7479000e+00 1.4906000e+00 3.6376000e-01 /
CHEB / -2.0640000e+00 2.7442000e-01 2.1315000e-01 /
CHEB / -1.2243000e+00 -1.1900000e-01 5.1497000e-02 /
CHEB / -6.2957000e-01 -1.6284000e-01 -2.4580000e-02 /

CH3CHO+C2H3(+m)=CH3CH[OH]CHcH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -13.1087457545981
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1594000e+00 3.7640000e-01 -1.3673000e-01 /
CHEB / 3.7481000e+00 1.1129000e+00 9.8671000e-02 /
CHEB / -1.5722000e+00 3.8729000e-01 2.0070000e-02 /
CHEB / -1.1179000e+00 3.7259000e-02 3.2151000e-02 /
CHEB / -6.3067000e-01 -9.6461000e-02 1.6392000e-02 /

CH3CHO+C2H3(+m)=CH3CH[OH]cCH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -15.308521234552533
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0219000e-01 5.6851000e-01 -1.3683000e-01 /
CHEB / 3.2687000e+00 1.2797000e+00 1.4839000e-01 /
CHEB / -1.7064000e+00 3.4005000e-01 6.2074000e-02 /
CHEB / -1.0622000e+00 -2.1274000e-02 2.7339000e-02 /
CHEB / -5.3680000e-01 -8.6733000e-02 -1.1075000e-03 /

CH3CHO+C2H3(+m)=CH3CH[o]C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H/Nd_O     Cd_pri_rad         deltaHrxn(T=298K)
= -20.247909158634773 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9741000e+00 2.1368000e+00 -4.9560000e-01 /
CHEB / -1.5219000e+00 5.9417000e-01 2.4535000e-01 /
CHEB / -2.6654000e+00 -1.7405000e-02 8.7249000e-02 /
CHEB / -1.3412000e+00 -1.9356000e-01 2.5484000e-03 /
CHEB / -5.3768000e-01 -1.2066000e-01 -1.7727000e-02 /

CH3CHO+C2H3(+m)=CH2CO+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -14.308726890368067
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0306000e-01 -1.1644000e+00 -5.0294000e-01 /
CHEB / 8.0586000e+00 1.3542000e+00 5.3665000e-01 /
CHEB / 5.1748000e-01 -1.5748000e-02 5.2580000e-02 /
CHEB / 4.5263000e-02 -1.4553000e-01 -5.2009000e-02 /
CHEB / -9.9671000e-03 -5.4511000e-02 -4.0856000e-02 /
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CH3CHO+C2H3(+m)=CH3CO+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -21.35767717708417
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6291000e-01 -6.3529000e-01 -3.8391000e-01 /
CHEB / 7.4259000e+00 7.7613000e-01 4.4838000e-01 /
CHEB / 3.3535000e-01 -4.9002000e-02 -3.1517000e-03 /
CHEB / 2.6299000e-02 -8.5948000e-02 -4.8863000e-02 /
CHEB / -3.0663000e-03 -2.1396000e-02 -1.9143000e-02 /

CH3CHO+C2H3(+m)=C4H6O(717)+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.259300021180422
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2306000e+00 -4.4168000e-01 -1.7636000e-01 /
CHEB / 2.9539000e+00 5.3618000e-01 1.9864000e-01 /
CHEB / -1.1585000e-01 -1.6373000e-02 1.5715000e-02 /
CHEB / -2.7244000e-03 -8.0821000e-02 -3.2815000e-02 /
CHEB / 6.6552000e-02 -2.1096000e-02 -1.5324000e-02 /

CH3CHO+C2H3(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -34.18670986066912
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4628000e+01 -2.6635000e-02 -1.8686000e-02 /
CHEB / 2.8365000e+01 2.7249000e-02 1.9105000e-02 /
CHEB / 1.0840000e+00 3.4222000e-03 2.4283000e-03 /
CHEB / 2.8302000e-01 -2.1898000e-03 -1.5431000e-03 /
CHEB / 5.7648000e-02 -1.9524000e-03 -1.3887000e-03 /

CH3CHO+C2H3(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.529218417633786
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5305000e+00 -6.3549000e-01 -3.5034000e-01 /
CHEB / 6.6047000e+00 7.7986000e-01 4.1439000e-01 /
CHEB / 3.8774000e-01 -6.9299000e-02 -1.5878000e-02 /
CHEB / 1.3057000e-01 -7.6502000e-02 -4.3814000e-02 /
CHEB / 5.2882000e-02 -1.0669000e-02 -1.1344000e-02 /

CH3CHO+C2H3(+m)=nC4H5+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -6.239838380070232
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9837000e+00 -2.8614000e-01 -1.6680000e-01 /
CHEB / 1.6939000e+01 3.0685000e-01 1.7012000e-01 /
CHEB / 3.8981000e-01 4.0054000e-02 3.2554000e-02 /
CHEB / 9.0171000e-02 -4.5464000e-02 -2.2135000e-02 /
CHEB / 3.4683000e-02 -2.5794000e-02 -1.7882000e-02 /
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CH3CHO+C2H3(+m)=CH3+C3H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -11.909229627866287
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7200000e+00 -4.4305000e-01 -1.7846000e-01 /
CHEB / 2.3399000e+00 5.3623000e-01 2.0016000e-01 /
CHEB / -3.3094000e-01 -1.3417000e-02 1.7003000e-02 /
CHEB / -1.1220000e-01 -8.1724000e-02 -3.2962000e-02 /
CHEB / 1.3269000e-03 -2.2501000e-02 -1.5999000e-02 /

C4H7-24+O(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -102.28955563021854
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1145000e+01 1.5401000e+01 -1.3897000e+00 /
CHEB / -3.9533000e+00 -4.4049000e-01 1.5602000e+00 /
CHEB / -2.4976000e+00 -1.2654000e+00 7.2478000e-01 /
CHEB / -1.6046000e+00 -6.0768000e-01 1.7654000e-01 /
CHEB / -8.5344000e-01 -2.3753000e-01 -6.6845000e-02 /

C4H7-24+O(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -102.28955563021854
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1856000e+01 1.4809000e+01 -1.3299000e+00 /
CHEB / -3.3260000e+00 -7.7814000e-02 1.4210000e+00 /
CHEB / -2.4438000e+00 -1.1187000e+00 7.2202000e-01 /
CHEB / -1.6257000e+00 -5.9962000e-01 2.0854000e-01 /
CHEB / -8.6999000e-01 -2.5530000e-01 -5.0952000e-02 /

C4H7-24+O(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -105.18922682545818
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0199000e+01 1.4570000e+01 -8.4267000e-01 /
CHEB / -4.7040000e+00 -1.7298000e-01 9.2145000e-01 /
CHEB / -2.7166000e+00 -9.9387000e-01 7.0725000e-01 /
CHEB / -1.6133000e+00 -5.4987000e-01 2.3926000e-01 /
CHEB / -8.4742000e-01 -2.2118000e-01 -3.4455000e-02 /

C4H7-24+O(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -104.98929724252075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8634000e+00 1.5042000e+01 -7.8620000e-01 /
CHEB / -4.1376000e+00 -5.0460000e-01 8.5873000e-01 /
CHEB / -2.4362000e+00 -1.0503000e+00 6.7786000e-01 /
CHEB / -1.5204000e+00 -5.5582000e-01 2.3764000e-01 /
CHEB / -8.3778000e-01 -2.2377000e-01 -2.9101000e-02 /
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C4H7-24+O(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -104.98929724252075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5807000e+00 1.3600000e+01 -1.0237000e+00 /
CHEB / -4.2934000e+00 -1.1831000e-01 1.1767000e+00 /
CHEB / -2.2861000e+00 -8.8905000e-01 6.9750000e-01 /
CHEB / -1.4141000e+00 -4.4076000e-01 2.4993000e-01 /
CHEB / -8.0540000e-01 -1.6053000e-01 -3.6673000e-02 /

C4H7-24+O(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -88.98086960152355
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2345000e+01 1.5743000e+01 -1.2949000e+00 /
CHEB / -4.6006000e+00 -5.5577000e-01 1.5213000e+00 /
CHEB / -2.7479000e+00 -1.4592000e+00 7.3919000e-01 /
CHEB / -1.5589000e+00 -7.7411000e-01 1.7243000e-01 /
CHEB / -6.9457000e-01 -2.9462000e-01 -7.8565000e-02 /

C4H7-24+O(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -78.88196831730295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3180000e+01 1.3934000e+01 2.6389000e-01 /
CHEB / -3.4671000e+00 -8.3722000e-01 1.2765000e+00 /
CHEB / -1.9879000e+00 -7.7419000e-01 1.7037000e-01 /
CHEB / -1.1401000e+00 -4.1700000e-01 4.9333000e-02 /
CHEB / -5.8804000e-01 -2.1498000e-01 -1.9444000e-02 /

C4H7-24+O(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -84.19148380939936
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2081000e+01 1.4337000e+01 -3.9587000e-01 /
CHEB / -3.7548000e+00 -7.6260000e-01 1.0179000e+00 /
CHEB / -2.2815000e+00 -8.3019000e-01 3.0896000e-01 /
CHEB / -1.3000000e+00 -5.4388000e-01 1.2370000e-01 /
CHEB / -6.2520000e-01 -2.9050000e-01 8.3513000e-03 /

C4H7-24+O(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -84.66126160155277
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0524000e+00 1.2582000e+01 -9.5942000e-01 /
CHEB / -3.7848000e+00 -1.1051000e+00 1.1031000e+00 /
CHEB / -2.4279000e+00 -9.9407000e-01 4.7871000e-01 /
CHEB / -1.4638000e+00 -4.5225000e-01 1.2683000e-01 /
CHEB / -8.1272000e-01 -1.2636000e-01 -4.2595000e-02 /
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C4H7-24+O(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -74.5623603177239
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9466000e+00 9.3831000e+00 -8.9378000e-01 /
CHEB / -3.4275000e+00 -5.9101000e-01 9.2795000e-01 /
CHEB / -2.5736000e+00 -5.2867000e-01 4.6431000e-01 /
CHEB / -1.4821000e+00 -3.2499000e-01 1.0594000e-01 /
CHEB / -8.0576000e-01 -1.0936000e-01 -3.9341000e-02 /

C4H7-24+O(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -76.76213579767834
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2540000e+00 1.1057000e+01 -5.6888000e-01 /
CHEB / -2.4921000e+00 -1.1242000e+00 9.2597000e-01 /
CHEB / -2.0117000e+00 -8.8627000e-01 5.9697000e-01 /
CHEB / -1.2066000e+00 -4.7883000e-01 1.3145000e-01 /
CHEB / -6.8735000e-01 -1.4156000e-01 -5.6474000e-02 /

C4H7-24+O(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: Oa_R_Recombination estimate:
(Average:) C_rad/H/OneDeC     Oa          deltaHrxn(T=298K) = -
81.70152372176058 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.6870000e+00 1.1339000e+01 -9.3532000e-01 /
CHEB / -3.8681000e+00 -6.5127000e-01 6.7406000e-01 /
CHEB / -2.9576000e+00 -8.4946000e-01 5.8446000e-01 /
CHEB / -1.6759000e+00 -5.1937000e-01 1.5706000e-01 /
CHEB / -8.2993000e-01 -1.9840000e-01 -2.2210000e-02 /

C4H7-24+O(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -75.76234145349386
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3851000e+00 -1.6901000e-02 -1.5493000e-02 /
CHEB / 2.0216000e+00 2.5852000e-02 2.3491000e-02 /
CHEB / 3.5631000e-01 -9.5016000e-03 -8.5698000e-03 /
CHEB / 2.5325000e-02 2.6802000e-04 2.7903000e-04 /
CHEB / -4.1858000e-02 5.8929000e-05 1.4653000e-04 /

C4H7-24+O(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -82.81129174020997
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7918000e+00 1.8956000e-02 1.2560000e-02 /
CHEB / 2.3498000e+00 -1.8407000e-02 -1.1796000e-02 /
CHEB / 3.7116000e-01 -2.6049000e-03 -2.2507000e-03 /
CHEB / 2.8172000e-03 8.3747000e-04 6.1313000e-04 /
CHEB / -6.0406000e-02 7.8128000e-04 5.4685000e-04 /
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C4H7-24+O(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -72.71291458430622
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6819000e+00 6.4822000e-05 4.4271000e-05 /
CHEB / 1.1851000e-01 -4.1847000e-05 -2.9238000e-05 /
CHEB / 4.5054000e-02 1.2213000e-05 9.5379000e-06 /
CHEB / 4.2307000e-02 5.5484000e-06 4.4439000e-06 /
CHEB / 2.5590000e-02 -1.4117000e-05 -1.0115000e-05 /

C4H7-24+O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -95.64032442379492
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4192000e+00 -6.4778000e-02 -4.2570000e-02 /
CHEB / 9.8048000e+00 7.4629000e-02 4.8430000e-02 /
CHEB / 1.8621000e+00 -9.9591000e-04 1.8000000e-04 /
CHEB / 4.6109000e-01 -7.3493000e-03 -4.8483000e-03 /
CHEB / 8.6465000e-02 -2.8588000e-03 -2.0784000e-03 /

C4H7-24+O(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -72.98283298075958
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1511000e+00 -5.9164000e-03 -4.5620000e-03 /
CHEB / 1.0864000e+00 5.8217000e-03 4.5240000e-03 /
CHEB / 2.7288000e-01 1.7387000e-03 1.2764000e-03 /
CHEB / 5.2615000e-02 -9.8551000e-04 -7.3530000e-04 /
CHEB / -1.6764000e-02 -1.0301000e-03 -7.9155000e-04 /

C4H7-24+O(+m)=C4H6-12+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -44.75567019063804
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2680000e+00 -8.7872000e-03 -6.0478000e-03 /
CHEB / 1.5877000e+00 6.4864000e-03 4.3583000e-03 /
CHEB / 5.3355000e-01 4.6596000e-03 3.3095000e-03 /
CHEB / 1.7184000e-01 -5.4749000e-04 -2.9061000e-04 /
CHEB / 2.7896000e-02 -1.8671000e-03 -1.3480000e-03 /

C4H7-24+O(+m)=C2H3O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -52.324658235913326
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9005000e+00 -4.1011000e-02 -3.3308000e-02 /
CHEB / 2.4174000e+00 5.4544000e-02 4.4741000e-02 /
CHEB / 5.2670000e-01 -1.1744000e-02 -1.0194000e-02 /
CHEB / 1.0345000e-01 -2.0081000e-03 -1.5586000e-03 /
CHEB / 1.9061000e-03 -1.7762000e-04 2.3184000e-05 /
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C4H7-24+O(+m)=HCCOH+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -41.83591580790841
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5460000e+00 -1.1732000e-01 -8.2554000e-02 /
CHEB / 2.5492000e+00 1.5227000e-01 1.0704000e-01 /
CHEB / 6.7290000e-01 -2.8851000e-02 -2.0017000e-02 /
CHEB / 1.0943000e-01 -5.9630000e-03 -4.4953000e-03 /
CHEB / -2.2911000e-02 -1.1326000e-03 -6.5266000e-04 /

C4H7-24+O(+m)=C4H6-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -43.70583454622083
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3767000e+00 -9.2726000e-02 -6.7062000e-02 /
CHEB / 3.2651000e+00 1.2252000e-01 8.8712000e-02 /
CHEB / 8.2223000e-01 -2.6120000e-02 -1.8959000e-02 /
CHEB / 1.6557000e-01 -3.6100000e-03 -2.7743000e-03 /
CHEB / 3.5802000e-03 -7.9119000e-04 -4.2036000e-04 /

C4H7-24+O(+m)=C4H6-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.02494516010884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3591000e+00 -1.8825000e-02 -1.3732000e-02 /
CHEB / 2.8406000e+00 1.9242000e-02 1.4252000e-02 /
CHEB / 8.3577000e-01 2.8210000e-03 1.7152000e-03 /
CHEB / 2.3331000e-01 -1.5430000e-03 -1.0266000e-03 /
CHEB / 4.4842000e-02 -1.9292000e-03 -1.3681000e-03 /

C4H7-24+O(+m)=C2H4O+C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.334885706658014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0332000e+00 -5.6610000e-02 -4.0134000e-02 /
CHEB / 2.6266000e+00 6.9889000e-02 4.9378000e-02 /
CHEB / 6.7819000e-01 -5.8818000e-03 -3.8239000e-03 /
CHEB / 1.7420000e-01 -8.0021000e-03 -5.8510000e-03 /
CHEB / 2.8855000e-02 -1.0227000e-03 -7.7757000e-04 /

C4H7-24+O(+m)=C4H6-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -56.77431176763851
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2134000e+00 -2.0529000e-02 -1.7566000e-02 /
CHEB / 1.0952000e+00 2.9968000e-02 2.5319000e-02 /
CHEB / 1.9038000e-01 -7.8471000e-03 -6.3345000e-03 /
CHEB / 2.0012000e-03 -3.4444000e-03 -2.9298000e-03 /
CHEB / -3.3651000e-02 9.8078000e-04 7.9787000e-04 /
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C4H7-24+O(+m)=C2H5O-2+C2H2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -51.23502076943023
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2595000e+00 -4.4628000e-02 -3.7147000e-02 /
CHEB / 4.9092000e-01 5.7102000e-02 4.6657000e-02 /
CHEB / 1.5925000e-02 -3.7235000e-03 -1.9747000e-03 /
CHEB / -1.0387000e-02 -1.1228000e-02 -9.1911000e-03 /
CHEB / -4.1928000e-03 -9.3533000e-04 -1.1858000e-03 /

C4H7-24+O(+m)=nC4H5+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -67.69345294319604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1916000e+00 -1.1114000e-01 -7.1844000e-02 /
CHEB / 3.2789000e+00 1.3086000e-01 8.3367000e-02 /
CHEB / 9.1106000e-01 -3.8545000e-04 1.4904000e-03 /
CHEB / 2.7940000e-01 -1.9712000e-02 -1.2738000e-02 /
CHEB / 8.9007000e-02 -4.0374000e-03 -3.2412000e-03 /

C4H7-24+O(+m)=CH3+C3H3OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -54.57487747273095
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3478000e+00 -5.9728000e-03 -4.1806000e-03 /
CHEB / 1.3721000e+00 3.8501000e-03 2.5960000e-03 /
CHEB / 4.5070000e-01 4.1122000e-03 2.9893000e-03 /
CHEB / 1.4265000e-01 -4.7447000e-04 -2.6891000e-04 /
CHEB / 1.9029000e-02 -1.6580000e-03 -1.2289000e-03 /

C4H7-24+O(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -73.36284419099209
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1058000e+01 6.6840000e-05 4.6537000e-05 /
CHEB / -4.8993000e-01 -6.7440000e-05 -4.6967000e-05 /
CHEB / -1.8479000e-01 -8.4493000e-06 -5.8665000e-06 /
CHEB / -7.3648000e-02 5.7415000e-06 4.0007000e-06 /
CHEB / -3.5584000e-02 3.3520000e-06 2.3272000e-06 /

C4H7-24+O(+m)=CH3CHO+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -61.45361456312581
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3013000e+01 -2.1138000e-06 -1.4787000e-06 /
CHEB / -2.7515000e-02 2.1473000e-06 1.4964000e-06 /
CHEB / -1.4346000e-02 9.7650000e-08 7.6081000e-08 /
CHEB / -6.6347000e-03 -1.4607000e-07 -1.0003000e-07 /
CHEB / -1.0110000e-02 -8.5458000e-08 -6.3154000e-08 /
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C4H7-22+O(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -121.18752607083233
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5694000e+01 1.9157000e+01 -9.9574000e-02 /
CHEB / -4.9385000e+00 -2.5294000e+00 1.6861000e+00 /
CHEB / -1.8467000e+00 -1.8986000e+00 -6.1090000e-02 /
CHEB / -1.1560000e+00 -9.0166000e-01 -1.7841000e-02 /
CHEB / -8.0466000e-01 -3.6234000e-01 2.0026000e-01 /

C4H7-22+O(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -121.18752607083233
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6527000e+01 1.8629000e+01 -2.0596000e-01 /
CHEB / -4.2691000e+00 -2.1800000e+00 1.6264000e+00 /
CHEB / -1.6906000e+00 -1.9108000e+00 8.3239000e-02 /
CHEB / -1.1903000e+00 -8.3379000e-01 -2.0571000e-02 /
CHEB / -8.4127000e-01 -3.3297000e-01 1.7929000e-01 /

C4H7-22+O(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: Oa_R_Recombination estimate:
(Average:) Cd_rad/NonDe     Oa      deltaHrxn(T=298K) = -
124.08719726607197 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5044000e+01 1.7624000e+01 4.4200000e-01 /
CHEB / -5.4953000e+00 -1.8193000e+00 1.1500000e+00 /
CHEB / -2.0434000e+00 -1.4249000e+00 -2.1417000e-01 /
CHEB / -1.1652000e+00 -7.4930000e-01 3.0309000e-02 /
CHEB / -7.9258000e-01 -2.9264000e-01 2.3407000e-01 /

C4H7-22+O(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -123.88726768313454
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4847000e+01 1.8164000e+01 3.4952000e-01 /
CHEB / -4.9247000e+00 -2.1940000e+00 1.1131000e+00 /
CHEB / -1.7488000e+00 -1.6359000e+00 -1.5652000e-01 /
CHEB / -1.0741000e+00 -8.0645000e-01 5.8801000e-02 /
CHEB / -7.7991000e-01 -2.9617000e-01 2.5402000e-01 /

C4H7-22+O(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -123.88726768313454
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3158000e+01 1.7270000e+01 2.5847000e-01 /
CHEB / -5.2894000e+00 -2.2999000e+00 1.3186000e+00 /
CHEB / -1.6157000e+00 -1.4869000e+00 -8.0828000e-02 /
CHEB / -9.6010000e-01 -6.4697000e-01 4.0029000e-02 /
CHEB / -7.5501000e-01 -2.6865000e-01 2.4209000e-01 /
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C4H7-22+O(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -107.87884004213734
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6278000e+01 1.8453000e+01 8.9606000e-01 /
CHEB / -5.6314000e+00 -2.5005000e+00 1.4965000e+00 /
CHEB / -2.3694000e+00 -1.6456000e+00 -4.1353000e-01 /
CHEB / -1.2771000e+00 -8.1312000e-01 -2.1952000e-01 /
CHEB / -7.2956000e-01 -2.6199000e-01 3.2010000e-02 /

C4H7-22+O(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -97.77993875791674
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6040000e+01 1.5137000e+01 2.6594000e+00 /
CHEB / -4.7579000e+00 -2.4944000e+00 7.3250000e-01 /
CHEB / -1.8969000e+00 -5.9761000e-01 -4.0772000e-01 /
CHEB / -9.8456000e-01 -3.0016000e-01 -2.3152000e-01 /
CHEB / -5.8865000e-01 -2.0318000e-01 1.0672000e-02 /

C4H7-22+O(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -103.08945425001315
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5844000e+01 1.5942000e+01 2.0142000e+00 /
CHEB / -4.8972000e+00 -2.0883000e+00 5.6528000e-01 /
CHEB / -1.9897000e+00 -7.7266000e-01 -5.3017000e-01 /
CHEB / -1.0550000e+00 -4.0827000e-01 -1.8270000e-01 /
CHEB / -5.6481000e-01 -2.7746000e-01 9.4578000e-03 /

C4H7-22+O(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -103.55923204216656
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2112000e+01 1.6485000e+01 8.3200000e-02 /
CHEB / -3.7935000e+00 -2.3791000e+00 8.2344000e-01 /
CHEB / -2.2300000e+00 -1.6266000e+00 1.5559000e-01 /
CHEB / -1.3168000e+00 -7.8519000e-01 1.3840000e-01 /
CHEB / -7.9418000e-01 -2.4066000e-01 1.1665000e-01 /

C4H7-22+O(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -93.46033075833769
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0025000e+01 1.3846000e+01 -4.1383000e-01 /
CHEB / -2.6778000e+00 -2.1909000e+00 9.2339000e-01 /
CHEB / -2.2930000e+00 -1.3717000e+00 4.7851000e-01 /
CHEB / -1.4371000e+00 -5.3602000e-01 7.8514000e-02 /
CHEB / -8.9056000e-01 -2.7748000e-02 -7.5978000e-02 /
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C4H7-22+O(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -95.66010623829213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3425000e+01 1.4409000e+01 9.3001000e-01 /
CHEB / -2.3914000e+00 -1.8858000e+00 1.7948000e-01 /
CHEB / -1.8967000e+00 -1.3627000e+00 1.2069000e-01 /
CHEB / -1.1240000e+00 -7.2845000e-01 1.3659000e-01 /
CHEB / -6.4391000e-01 -2.7621000e-01 1.1128000e-01 /

C4H7-22+O(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -100.59949416237437
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6718000e+01 1.5721000e+01 -3.7599000e-01 /
CHEB / -3.1668000e+00 -2.1736000e+00 5.9839000e-01 /
CHEB / -2.7398000e+00 -1.5715000e+00 5.0374000e-01 /
CHEB / -1.6361000e+00 -7.2266000e-01 1.2711000e-01 /
CHEB / -8.9518000e-01 -1.5533000e-01 -2.2168000e-02 /

C4H7-22+O(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -94.66031189410765
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0320000e+01 8.7485000e-04 6.1607000e-04 /
CHEB / 1.0575000e+00 -1.1296000e-03 -7.9607000e-04 /
CHEB / 7.6079000e-02 2.4930000e-04 1.7526000e-04 /
CHEB / -2.5302000e-02 3.2169000e-05 2.4758000e-05 /
CHEB / -2.3400000e-02 -2.8204000e-05 -2.1586000e-05 /

C4H7-22+O(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -101.70926218082376
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0308000e+01 2.4574000e-04 1.7363000e-04 /
CHEB / 1.2272000e+00 -2.0842000e-04 -1.4856000e-04 /
CHEB / 8.5671000e-02 -5.1866000e-05 -3.5242000e-05 /
CHEB / -5.3185000e-02 3.1304000e-06 2.2660000e-06 /
CHEB / -4.9919000e-02 9.3855000e-06 6.4732000e-06 /

C4H7-22+O(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -91.61088502492001
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1990000e+01 5.4425000e-05 3.7948000e-05 /
CHEB / 5.1287000e-01 -4.8913000e-05 -3.4110000e-05 /
CHEB / 8.3446000e-02 -1.1970000e-05 -8.3495000e-06 /
CHEB / 2.9182000e-02 2.8149000e-06 1.9759000e-06 /
CHEB / 1.1316000e-02 3.0902000e-06 2.1524000e-06 /
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C4H7-22+O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -114.53829486440871
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0942000e+00 -2.5600000e-03 -1.7696000e-03 /
CHEB / 5.8107000e+00 2.3152000e-03 1.5947000e-03 /
CHEB / 1.6770000e+00 5.6335000e-04 3.9615000e-04 /
CHEB / 4.8961000e-01 -1.6792000e-04 -1.1586000e-04 /
CHEB / 1.2395000e-01 -1.4383000e-04 -1.0044000e-04 /

C4H7-22+O(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -91.88080342137337
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2952000e+01 -3.9878000e-06 -2.7862000e-06 /
CHEB / -1.3453000e-01 7.2871000e-07 5.2462000e-07 /
CHEB / -6.2519000e-02 1.9329000e-06 1.3344000e-06 /
CHEB / -1.8199000e-02 9.3764000e-07 6.5745000e-07 /
CHEB / -8.0489000e-03 5.5874000e-08 3.8546000e-08 /

C4H7-22+O(+m)=C4H6-12+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -63.65364063125183
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2011000e+00 -5.8992000e-03 -4.1731000e-03 /
CHEB / 9.4143000e-01 7.7689000e-03 5.5136000e-03 /
CHEB / 3.2834000e-01 -1.7576000e-03 -1.2742000e-03 /
CHEB / 1.3466000e-01 -1.3698000e-04 -8.2739000e-05 /
CHEB / 4.7080000e-02 -1.6941000e-06 -1.6298000e-06 /

C4H7-22+O(+m)=C2H3O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -71.22262867652711
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6959000e+00 3.4542000e-04 2.1760000e-04 /
CHEB / 1.5097000e+00 -5.5816000e-04 -3.5060000e-04 /
CHEB / 2.6351000e-01 1.7093000e-04 9.6331000e-05 /
CHEB / 6.4233000e-02 8.4166000e-05 6.9261000e-05 /
CHEB / 2.4740000e-02 -3.6808000e-05 -2.9363000e-05 /

C4H7-22+O(+m)=HCCOH+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -60.7338862485222
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8703000e+00 -1.4373000e-02 -1.0213000e-02 /
CHEB / 1.2975000e+00 1.9227000e-02 1.3713000e-02 /
CHEB / 3.2169000e-01 -4.9098000e-03 -3.5758000e-03 /
CHEB / 6.0660000e-02 1.7625000e-04 1.6570000e-04 /
CHEB / 4.9615000e-03 -1.1800000e-04 -8.7510000e-05 /
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C4H7-22+O(+m)=C4H6-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -62.60380498683462
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5319000e+00 -8.5595000e-03 -6.1540000e-03 /
CHEB / 2.1245000e+00 1.1615000e-02 8.3986000e-03 /
CHEB / 4.9837000e-01 -3.1987000e-03 -2.3849000e-03 /
CHEB / 1.1552000e-01 2.4310000e-04 2.1840000e-04 /
CHEB / 2.7492000e-02 -9.1071000e-05 -7.2292000e-05 /

C4H7-22+O(+m)=C4H6-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -69.92291560072265
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6441000e+00 4.3143000e-04 3.0026000e-04 /
CHEB / 1.5433000e+00 -5.8397000e-04 -4.0647000e-04 /
CHEB / 3.7773000e-01 1.0422000e-04 7.2289000e-05 /
CHEB / 1.4960000e-01 6.6721000e-05 4.7081000e-05 /
CHEB / 6.6657000e-02 -3.9054000e-06 -3.1412000e-06 /

C4H7-22+O(+m)=C2H4O+C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -70.23285614727182
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3370000e+00 -2.4949000e-02 -1.7869000e-02 /
CHEB / 2.3417000e+00 3.0674000e-02 2.2048000e-02 /
CHEB / 4.6597000e-01 -3.1389000e-03 -2.3551000e-03 /
CHEB / 9.6063000e-02 -2.5144000e-03 -1.7963000e-03 /
CHEB / 1.4882000e-02 -4.6921000e-04 -3.1104000e-04 /

C4H7-22+O(+m)=C4H6-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -75.6722822082523
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2537000e+00 -5.4488000e-03 -4.1138000e-03 /
CHEB / 9.7326000e-01 8.0988000e-03 6.1365000e-03 /
CHEB / 3.4659000e-02 -2.4278000e-03 -1.8981000e-03 /
CHEB / -6.7704000e-02 -4.6379000e-04 -3.1179000e-04 /
CHEB / -4.9612000e-02 1.0303000e-04 9.5470000e-05 /

C4H7-22+O(+m)=C2H5O-2+C2H2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -70.13299121004403
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6313000e+00 -9.0278000e-03 -6.7395000e-03 /
CHEB / 1.0300000e+00 1.2144000e-02 9.0983000e-03 /
CHEB / 1.1095000e-01 -2.4859000e-03 -1.8834000e-03 /
CHEB / -6.7216000e-03 -1.0729000e-03 -8.3442000e-04 /
CHEB / -1.2786000e-02 2.9313000e-04 2.4503000e-04 /
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C4H7-22+O(+m)=nC4H5+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -86.59142338380983
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2974000e+00 -4.3696000e-02 -3.0663000e-02 /
CHEB / 3.3338000e+00 5.1267000e-02 3.5984000e-02 /
CHEB / 8.6243000e-01 -1.4096000e-03 -9.8026000e-04 /
CHEB / 2.6605000e-01 -5.8241000e-03 -4.1152000e-03 /
CHEB / 8.5110000e-02 -1.3627000e-03 -9.5468000e-04 /

C4H7-22+O(+m)=CH3+C3H3OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -73.47284791334474
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2214000e+00 -9.8148000e-03 -6.9334000e-03 /
CHEB / 1.6946000e+00 1.1063000e-02 7.8230000e-03 /
CHEB / 3.3441000e-01 1.6269000e-04 1.1040000e-04 /
CHEB / 4.9755000e-02 -1.0576000e-03 -7.5562000e-04 /
CHEB / -8.0602000e-03 -5.1049000e-04 -3.5895000e-04 /

C4H7-22+O(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -92.26081463160587
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6836000e+00 -1.0112000e-02 -7.1304000e-03 /
CHEB / 1.1308000e+00 1.0620000e-02 7.5009000e-03 /
CHEB / 2.6382000e-01 1.1182000e-03 7.7935000e-04 /
CHEB / 5.0572000e-02 -1.0448000e-03 -7.4607000e-04 /
CHEB / -2.2185000e-03 -6.9210000e-04 -4.8548000e-04 /

C4H7-22+O(+m)=CH3CHO+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -80.3515850037396
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7659000e+00 -1.3282000e-02 -9.3046000e-03 /
CHEB / 1.5455000e+00 1.3794000e-02 9.6636000e-03 /
CHEB / 4.1098000e-01 1.6284000e-03 1.1473000e-03 /
CHEB / 1.0873000e-01 -1.3248000e-03 -9.3581000e-04 /
CHEB / 2.0269000e-02 -9.5020000e-04 -6.6828000e-04 /

C4H7-22+O(+m)=C4H7-24+O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -18.897970440613797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0734000e-01 -3.7001000e-02 -2.4884000e-02 /
CHEB / 3.5516000e+00 4.1317000e-02 2.7575000e-02 /
CHEB / 1.2241000e+00 1.5866000e-03 1.3389000e-03 /
CHEB / 3.6660000e-01 -4.6370000e-03 -3.0913000e-03 /
CHEB / 8.4134000e-02 -2.2393000e-03 -1.5912000e-03 /

C4H7-12+O(+m)=cH2C[O]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5) High-P Limit: Oa_R_Recombination estimate:
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(Average:) Cd_rad/NonDe     Oa      deltaHrxn(T=298K) = -
124.297266129318 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4753000e+01 1.9063000e+01 5.0234000e-01 /
CHEB / -5.0539000e+00 -2.3122000e+00 1.1228000e+00 /
CHEB / -1.9937000e+00 -1.7871000e+00 -1.8818000e-01 /
CHEB / -1.2404000e+00 -1.0148000e+00 3.2966000e-02 /
CHEB / -8.2997000e-01 -3.6403000e-01 2.2645000e-01 /

C4H7-12+O(+m)=CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -124.297266129318
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5842000e+01 1.9007000e+01 -1.3117000e-02 /
CHEB / -4.1531000e+00 -2.4040000e+00 1.4406000e+00 /
CHEB / -1.7930000e+00 -1.8742000e+00 2.4200000e-02 /
CHEB / -1.2587000e+00 -9.6908000e-01 5.1370000e-02 /
CHEB / -8.7390000e-01 -3.2182000e-01 1.9362000e-01 /

C4H7-12+O(+m)=CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -127.19693732455764
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4715000e+01 1.8292000e+01 1.2141000e-01 /
CHEB / -5.1989000e+00 -2.1537000e+00 1.2833000e+00 /
CHEB / -1.8744000e+00 -1.7588000e+00 9.7628000e-02 /
CHEB / -1.2544000e+00 -7.0573000e-01 5.4368000e-03 /
CHEB / -8.7571000e-01 -2.5397000e-01 1.7745000e-01 /

C4H7-12+O(+m)=CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -126.99700774162021
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4458000e+01 1.8599000e+01 1.4074000e-01 /
CHEB / -4.6418000e+00 -2.4380000e+00 1.2336000e+00 /
CHEB / -1.6533000e+00 -1.8050000e+00 2.8455000e-02 /
CHEB / -1.1626000e+00 -7.3816000e-01 2.6628000e-02 /
CHEB / -8.5430000e-01 -2.6249000e-01 2.0814000e-01 /

C4H7-12+O(+m)=CH2C[OH]cHCH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -126.99700774162021
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2520000e+01 1.7609000e+01 3.8497000e-01 /
CHEB / -5.1143000e+00 -2.4819000e+00 1.2267000e+00 /
CHEB / -1.7135000e+00 -1.5068000e+00 -1.4152000e-01 /
CHEB / -1.0429000e+00 -7.0222000e-01 7.6653000e-02 /
CHEB / -7.9364000e-01 -2.6357000e-01 2.5080000e-01 /

C4H7-12+O(+m)=CH2C[OH]CH2cH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -110.98858010062301
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5407000e+01 1.8455000e+01 1.3264000e+00 /
CHEB / -5.6407000e+00 -2.3567000e+00 1.0779000e+00 /
CHEB / -2.5058000e+00 -1.6733000e+00 -4.2554000e-01 /
CHEB / -1.3994000e+00 -8.4714000e-01 -1.7697000e-01 /
CHEB / -7.2788000e-01 -2.9306000e-01 3.9864000e-02 /

C4H7-12+O(+m)=cHC[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -100.88967881640241
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4653000e+01 1.4826000e+01 3.2287000e+00 /
CHEB / -5.2917000e+00 -2.3146000e+00 1.7672000e-01 /
CHEB / -1.9516000e+00 -3.9426000e-01 -3.7883000e-01 /
CHEB / -1.0854000e+00 -3.9159000e-01 -1.9973000e-01 /
CHEB / -6.1259000e-01 -2.5178000e-01 -1.1099000e-02 /

C4H7-12+O(+m)=CH3C[OH]cCH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -106.19919430849882
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5466000e+01 1.6589000e+01 1.9497000e+00 /
CHEB / -4.6871000e+00 -2.3713000e+00 5.8618000e-01 /
CHEB / -1.9161000e+00 -9.3285000e-01 -5.3043000e-01 /
CHEB / -1.0888000e+00 -4.5054000e-01 -1.6477000e-01 /
CHEB / -5.9149000e-01 -3.0787000e-01 2.1357000e-02 /

C4H7-12+O(+m)=cH2CH[OH]C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -106.66897210065223
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2627000e+01 1.6851000e+01 2.1897000e-01 /
CHEB / -3.0569000e+00 -2.5265000e+00 7.3879000e-01 /
CHEB / -2.0473000e+00 -1.6598000e+00 1.2270000e-01 /
CHEB / -1.2772000e+00 -8.0278000e-01 1.5227000e-01 /
CHEB / -7.8445000e-01 -2.5449000e-01 1.3607000e-01 /

C4H7-12+O(+m)=CH3CH[OH]CHcH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -96.57007081682336
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0600000e+01 1.4283000e+01 -3.4386000e-01 /
CHEB / -1.9218000e+00 -2.3938000e+00 8.7484000e-01 /
CHEB / -2.0945000e+00 -1.4443000e+00 4.7941000e-01 /
CHEB / -1.4042000e+00 -5.4302000e-01 8.5593000e-02 /
CHEB / -8.8752000e-01 -2.3760000e-02 -7.0727000e-02 /

C4H7-12+O(+m)=CH3CH[OH]cCH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -98.7698462967778
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -1.3919000e+01 1.4765000e+01 1.0825000e+00 /
CHEB / -1.6776000e+00 -2.0594000e+00 8.6908000e-02 /
CHEB / -1.7122000e+00 -1.3747000e+00 9.1819000e-02 /
CHEB / -1.0930000e+00 -7.3478000e-01 1.3628000e-01 /
CHEB / -6.3520000e-01 -2.8170000e-01 1.1927000e-01 /

C4H7-12+O(+m)=CH3CH[o]C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -103.70923422086004
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7249000e+01 1.6090000e+01 -2.3428000e-01 /
CHEB / -2.4524000e+00 -2.3257000e+00 4.8291000e-01 /
CHEB / -2.5585000e+00 -1.5937000e+00 4.7673000e-01 /
CHEB / -1.5967000e+00 -7.4993000e-01 1.4488000e-01 /
CHEB / -8.7922000e-01 -1.7370000e-01 3.9198000e-03 /

C4H7-12+O(+m)=CH2CO+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -97.77005195259332
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2856000e+01 -7.8672000e-06 -5.4151000e-06 /
CHEB / -3.7440000e-01 2.3730000e-05 1.6430000e-05 /
CHEB / -1.9015000e-01 6.4858000e-06 4.5628000e-06 /
CHEB / -9.3153000e-02 -1.1377000e-05 -7.9305000e-06 /
CHEB / -4.6028000e-02 -1.1092000e-05 -7.7433000e-06 /

C4H7-12+O(+m)=CH3CO+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -104.81900223930943
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1408000e+01 1.3277000e-03 9.3050000e-04 /
CHEB / 1.6798000e-01 -1.0120000e-03 -7.1058000e-04 /
CHEB / -1.2465000e-01 -4.1913000e-04 -2.9318000e-04 /
CHEB / -8.7444000e-02 2.4897000e-07 9.4929000e-07 /
CHEB / -4.5139000e-02 6.9459000e-05 4.8922000e-05 /

C4H7-12+O(+m)=C4H6O(717)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -94.72062508340568
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1019000e+01 1.2899000e-03 9.1212000e-04 /
CHEB / 1.1948000e+00 -1.4662000e-03 -1.0403000e-03 /
CHEB / 1.4991000e-01 8.3830000e-05 6.3422000e-05 /
CHEB / 9.0627000e-03 6.3214000e-05 4.5178000e-05 /
CHEB / -1.0044000e-02 2.1573000e-05 1.4029000e-05 /

C4H7-12+O(+m)=C3H7-1+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -117.64803492289438
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2999000e+00 -1.0863000e-02 -7.5207000e-03 /
CHEB / 4.5359000e+00 1.1018000e-02 7.6185000e-03 /
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CHEB / 1.4486000e+00 1.5210000e-03 1.0617000e-03 /
CHEB / 4.5438000e-01 -1.2176000e-03 -8.3902000e-04 /
CHEB / 1.3555000e-01 -5.7203000e-04 -3.9820000e-04 /

C4H7-12+O(+m)=CH3+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -94.99054347985904
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1941000e+01 -2.7868000e-04 -2.0011000e-04 /
CHEB / 5.4499000e-01 2.0829000e-04 1.5461000e-04 /
CHEB / 8.4288000e-03 9.4874000e-05 6.1054000e-05 /
CHEB / -3.3452000e-02 1.2116000e-05 1.0599000e-05 /
CHEB / -2.6257000e-02 -3.0074000e-05 -2.1789000e-05 /

C4H7-12+O(+m)=C4H6-12+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -66.7633806897375
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0239000e+01 -7.1685000e-03 -5.0633000e-03 /
CHEB / 5.9884000e-01 8.4734000e-03 6.0083000e-03 /
CHEB / 1.5510000e-01 -8.0098000e-04 -6.0081000e-04 /
CHEB / 4.3489000e-02 -3.2912000e-04 -2.2273000e-04 /
CHEB / 8.3199000e-03 -1.8164000e-04 -1.2630000e-04 /

C4H7-12+O(+m)=C2H3O-2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -74.33236873501278
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1545000e+01 2.9114000e-04 2.0209000e-04 /
CHEB / 4.0036000e-01 -4.0003000e-04 -2.7836000e-04 /
CHEB / 6.1396000e-02 1.0974000e-05 8.1109000e-06 /
CHEB / 7.3761000e-03 9.2409000e-05 6.4685000e-05 /
CHEB / -3.8831000e-03 2.8640000e-05 1.9692000e-05 /

C4H7-12+O(+m)=HCCOH+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -63.84362630700787
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2732000e+00 -8.4067000e-03 -5.9389000e-03 /
CHEB / 3.9201000e-03 1.0459000e-02 7.4156000e-03 /
CHEB / -2.4058000e-04 -1.6657000e-03 -1.2205000e-03 /
CHEB / -1.2594000e-02 -2.5764000e-04 -1.6407000e-04 /
CHEB / -1.7914000e-02 -1.3416000e-04 -9.5519000e-05 /

C4H7-12+O(+m)=C4H6-1+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -65.71354504532029
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0926000e+01 -4.5250000e-03 -3.2259000e-03 /
CHEB / 8.4568000e-01 5.5571000e-03 3.9868000e-03 /
CHEB / 1.7897000e-01 -7.7391000e-04 -5.9409000e-04 /
CHEB / 4.3407000e-02 -1.6454000e-04 -9.9115000e-05 /
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CHEB / 4.7204000e-03 -9.5418000e-05 -6.9338000e-05 /

C4H7-12+O(+m)=C4H6-2+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -73.03265565920832
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9194000e+00 8.1415000e-04 5.6674000e-04 /
CHEB / 1.7077000e+00 -1.3388000e-03 -9.3183000e-04 /
CHEB / 3.7692000e-01 5.4141000e-04 3.7510000e-04 /
CHEB / 9.5343000e-02 6.8624000e-05 5.1408000e-05 /
CHEB / 2.8549000e-02 -6.1017000e-05 -4.5014000e-05 /

C4H7-12+O(+m)=C2H4O+C2H3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -73.34259620575749
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1516000e+00 -3.2654000e-02 -2.3495000e-02 /
CHEB / 2.7388000e+00 4.0221000e-02 2.9073000e-02 /
CHEB / 4.8644000e-01 -4.5266000e-03 -3.4471000e-03 /
CHEB / 6.2367000e-02 -2.8497000e-03 -2.0272000e-03 /
CHEB / -1.0232000e-02 -6.0927000e-04 -4.0361000e-04 /

C4H7-12+O(+m)=C4H6-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -78.78202226673797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0604000e+00 -8.8652000e-03 -6.6302000e-03 /
CHEB / 1.3928000e+00 1.2657000e-02 9.5198000e-03 /
CHEB / 6.2643000e-02 -3.3800000e-03 -2.6488000e-03 /
CHEB / -9.8423000e-02 -5.9013000e-04 -3.8398000e-04 /
CHEB / -7.4261000e-02 8.3185000e-06 2.8736000e-05 /

C4H7-12+O(+m)=C2H5O-2+C2H2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -73.2427312685297
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4409000e+00 -1.5686000e-02 -1.1525000e-02 /
CHEB / 1.4320000e+00 2.0525000e-02 1.5162000e-02 /
CHEB / 1.3127000e-01 -3.8714000e-03 -2.9448000e-03 /
CHEB / -4.1546000e-02 -1.3135000e-03 -9.8486000e-04 /
CHEB / -3.8990000e-02 1.6957000e-04 1.5995000e-04 /

C4H7-12+O(+m)=nC4H5+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -89.7011634422955
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1296000e+00 -5.8120000e-02 -4.1000000e-02 /
CHEB / 3.6820000e+00 6.8988000e-02 4.8738000e-02 /
CHEB / 8.7003000e-01 -3.8277000e-03 -2.7770000e-03 /
CHEB / 2.2791000e-01 -6.5517000e-03 -4.6474000e-03 /
CHEB / 6.0038000e-02 -1.5310000e-03 -1.0565000e-03 /
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C4H7-12+O(+m)=CH3+C3H3OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -76.5825879718304
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0310000e+00 -1.6003000e-02 -1.1399000e-02 /
CHEB / 2.0987000e+00 1.8636000e-02 1.3323000e-02 /
CHEB / 3.5486000e-01 -8.1302000e-04 -6.4505000e-04 /
CHEB / 1.5658000e-02 -1.3415000e-03 -9.4886000e-04 /
CHEB / -3.3480000e-02 -6.5234000e-04 -4.5693000e-04 /

C4H7-12+O(+m)=CH3+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -95.37055469009154
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4889000e+00 -1.5042000e-02 -1.0690000e-02 /
CHEB / 1.5355000e+00 1.6305000e-02 1.1640000e-02 /
CHEB / 2.8071000e-01 7.6123000e-04 4.7215000e-04 /
CHEB / 1.4310000e-02 -1.2619000e-03 -8.9320000e-04 /
CHEB / -2.8501000e-02 -8.6573000e-04 -6.0737000e-04 /

C4H7-12+O(+m)=CH3CHO+C2H3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -83.46132506222527
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5745000e+00 -2.0393000e-02 -1.4405000e-02 /
CHEB / 1.9399000e+00 2.2142000e-02 1.5688000e-02 /
CHEB / 4.2422000e-01 9.2194000e-04 5.8929000e-04 /
CHEB / 7.1133000e-02 -1.6593000e-03 -1.1671000e-03 /
CHEB / -6.1352000e-03 -1.1451000e-03 -8.0398000e-04 /

C4H7-12+O(+m)=C4H7-24+O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -22.007710499099467
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7662000e-01 -6.2119000e-02 -4.2324000e-02 /
CHEB / 3.8098000e+00 7.3380000e-02 4.9817000e-02 /
CHEB / 1.2184000e+00 -3.7726000e-03 -2.3353000e-03 /
CHEB / 3.2812000e-01 -6.4292000e-03 -4.3719000e-03 /
CHEB / 6.3200000e-02 -2.2237000e-03 -1.5723000e-03 /

C4H7-12+O(+m)=C4H7-22+O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (cH2C[O]C2H5)  deltaHrxn(T=298K) = -3.10974005848567
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0789000e+00 -2.1738000e-02 -1.4827000e-02 /
CHEB / 4.7924000e+00 2.7436000e-02 1.8621000e-02 /
CHEB / 1.3836000e+00 -4.0402000e-03 -2.5936000e-03 /
CHEB / 3.7057000e-01 -1.9053000e-03 -1.3715000e-03 /
CHEB / 8.8395000e-02 2.6937000e-05 1.5820000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
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!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(447)         -37.64      89.34 27.54 33.25 38.23 42.04 48.77
      53.38 59.21 null
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!Here are the path reactions and their high-P limit kinetics:
!     CH3CHO+CH2CHO=nSPC(447) 7.9400000e+10      0.00000
6.7000000e+03

nSPC(447)(+m)=CH3CHO+CH2CHO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (nSPC(447))    deltaHrxn(T=298K) = 3.150007649495948
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6895000e+00 1.9268000e+00 -4.2067000e-02 /
CHEB / -7.8260000e-01 5.3336000e-03 1.3088000e-02 /
CHEB / -2.3252000e+00 2.6354000e-02 1.9438000e-02 /
CHEB / -1.0236000e+00 9.4086000e-03 5.0151000e-03 /
CHEB / -4.5709000e-01 2.5179000e-05 -1.0870000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -38.0 94.01 26.13 31.71 36.76 40.86 47.54 52.26
      55.9  null
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol2+HCO=unknown1(1)         5.2000000e+11      0.00000
6.5600000e+03
!     C3H4O+CH2OH=unknown1(1)       7.2517543e+09      0.48800
1.0375000e+04
!     C3H7O-N1+CO=unknown1(1)       4.0416992e+07      1.70125
8.2775000e+04

C3H6O-enol2+HCO(+m)=C3H7O-N1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown1)     deltaHrxn(T=298K) = -18.55799554756279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -1.3913000e+01 1.1084000e-05 7.4338000e-06 /
CHEB / 2.2402000e+01 -3.7402000e-06 -2.1586000e-06 /
CHEB / 1.3578000e-01 -6.5172000e-06 -4.7168000e-06 /
CHEB / 3.8017000e-02 -1.1152000e-06 -7.9081000e-07 /
CHEB / -9.1587000e-03 7.0437000e-07 5.2620000e-07 /

C3H4O+CH2OH(+m)=C3H6O-enol2+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown1)     deltaHrxn(T=298K) = -0.8101938213968278
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4577000e+00 -7.4832000e-01 -1.4937000e-01 /
CHEB / 4.3696000e+00 8.9589000e-01 1.2581000e-01 /
CHEB / -9.6074000e-02 -2.1201000e-02 7.3461000e-02 /
CHEB / -1.0146000e-01 -1.2468000e-01 -2.9041000e-02 /
CHEB / -3.7014000e-02 -3.4372000e-02 -3.0233000e-02 /

C3H4O+CH2OH(+m)=C3H7O-N1+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown1)     deltaHrxn(T=298K) = -19.36818936895962
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4659000e+01 -8.2875000e-04 -5.8256000e-04 /
CHEB / 2.2618000e+01 8.9692000e-04 6.3170000e-04 /
CHEB / 2.5442000e-01 4.8993000e-05 3.3051000e-05 /
CHEB / 7.2830000e-02 -8.9634000e-05 -6.3234000e-05 /
CHEB / 6.5403000e-03 -3.5938000e-05 -2.4956000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -61.63      82.58 26.48 32.32 37.23 41.27 47.98
      52.73 58.5  null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CO2               -94.36      50.99 8.87  9.84  10.63 11.26 12.23
      12.9  13.82
!     C4H7OJ(8)         -12.53      83.27 24.09 28.93 33.21 36.9  43.23
      47.78 53.46 null
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+CO2=unknown1(1)        1.9263655e+11      0.04067
9.2900000e+03
!     C4H7OJ(8)+O=unknown1(1)       1.0000000e+13      0.00000
0.0000000e+00

C4H7OJ(8)+O(+m)=C3H7-1+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (unknown1)     deltaHrxn(T=298K) = -116.24778509737355
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3748000e+01 3.0745000e-09 2.1401000e-09 /
CHEB / -6.1205000e-01 5.9584000e-09 4.1475000e-09 /
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CHEB / -5.2645000e-03 5.4302000e-09 3.7798000e-09 /
CHEB / 7.7747000e-03 4.6574000e-09 3.2419000e-09 /
CHEB / 5.2167000e-04 3.7453000e-09 2.6070000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -33.74      81.54 24.94 31.82 37.45 41.91 48.62
      53.73 59.36 null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH2CHO            6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34
      26.35  Neither TRange included 298K!
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!Here are the path reactions and their high-P limit kinetics:
!     C2H5+CH2CHO=unknown2(2)       1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4+C2H4O=unknown2(2)        1.1691492e+02      2.87714
4.8857143e+04

C2H5+CH2CHO(+m)=C2H4+C2H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (unknown2)     deltaHrxn(T=298K) = -50.991760108989006
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6639000e+00 -1.2777000e+00 -6.1375000e-02 /
CHEB / 3.5251000e+00 1.0589000e+00 -3.1820000e-02 /
CHEB / 4.5626000e-01 3.9211000e-01 6.3975000e-02 /
CHEB / -8.9966000e-02 -9.7941000e-03 5.4088000e-02 /
CHEB / -7.1990000e-02 -1.0108000e-01 6.0832000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -28.55      73.68 20.8  27.7  34.11 39.08 46.96
      52.54 63.11 null
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CH2O        -26.22      52.16 8.44  9.33  10.38 11.42 13.25 14.69
      16.9
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     CH3CHO+C2H4=unknown3(3)       2.3300000e+06      1.65000
5.4150000e+04
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!     CH2O+C3H6=unknown3(3)   6.9200000e+10      0.00000
4.3720000e+04

CH2O+C3H6(+m)=CH3CHO+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #14 (unknown3)    deltaHrxn(T=298K) = -5.709313590750673
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0723000e+01 -1.1823000e+00 -8.6404000e-02 /
CHEB / 1.8537000e+01 1.0715000e+00 -8.5603000e-03 /
CHEB / 1.4494000e-01 3.1095000e-01 8.9522000e-02 /
CHEB / -1.6771000e-01 -6.0148000e-02 4.8708000e-02 /
CHEB / -9.2640000e-02 -1.0603000e-01 -9.4907000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       -69.54      92.18 28.04 35.33 41.17 45.78 52.73
      57.9  61.55 null
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     CH2CHO            6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34
      26.35  Neither TRange included 298K!
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!Here are the path reactions and their high-P limit kinetics:
!     C2H5O-1+CH2CHO=unknown4(4)    1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4O+C2H4O=unknown4(4)       1.1691492e+02      2.87714
4.8857143e+04

C2H5O-1+CH2CHO(+m)=C2H4O+C2H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (unknown4)    deltaHrxn(T=298K) = -58.4410124183951
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4962000e+00 -1.3271000e+00 -5.3637000e-02 /
CHEB / 2.5405000e+00 1.0297000e+00 -3.6170000e-02 /
CHEB / 3.0641000e-01 4.4101000e-01 5.0455000e-02 /
CHEB / -1.4047000e-01 3.6947000e-02 5.3873000e-02 /
CHEB / -1.2246000e-01 -9.1103000e-02 1.4235000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -75.05      92.42 27.32 34.06 39.71 44.06 51.11
      56.07 61.04 null
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
```

```
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!Here are the path reactions and their high-P limit kinetics:
!     CH2OH+C3H5O-enol2=unknown5(5) 4.7900000e+14      -0.75000
0.0000000e+00
!     C2H4O+C2H4O=unknown5(5)       1.6297242e+02      2.92024
4.4628571e+04

CH2OH+C3H5O-enol2(+m)=C2H4O+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #34 (unknown5)     deltaHrxn(T=298K) = -
53.01462606880242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1921000e+00 -1.3912000e+00 -5.1713000e-02 /
CHEB / 3.1740000e+00 1.0044000e+00 -5.3377000e-02 /
CHEB / 4.4338000e-01 5.2955000e-01 3.7526000e-02 /
CHEB / -1.9113000e-01 1.0229000e-01 7.6405000e-02 /
CHEB / -1.7382000e-01 -1.0365000e-01 4.4131000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -88.13      90.52 27.49 33.98 39.74 44.22 51.55
      56.72 62.49 null
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!Here are the path reactions and their high-P limit kinetics:
!     C4H7OJ(12)+OH=unknown6(6)     1.4157154e+13      -0.15000
2.9166667e+02
!     CH3OH+C3H4O=unknown6(6) 1.6297242e+02      2.92024
4.4628571e+04

C4H7OJ(12)+OH(+m)=CH3OH+C3H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (unknown6)    deltaHrxn(T=298K) = -65.01308188534813
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7718000e+00 -1.2797000e+00 -7.2702000e-02 /
CHEB / 2.4312000e+00 1.0799000e+00 -4.3986000e-02 /
CHEB / 2.6081000e-01 4.1516000e-01 8.1245000e-02 /
CHEB / -1.7234000e-01 -2.7307000e-02 8.2627000e-02 /
CHEB / -1.3122000e-01 -1.3429000e-01 1.0932000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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```
!     unknown1(1)       -85.23      92.79 28.02 33.87 38.89 43.19 50.5
      55.68 60.29 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H5OJ(13)        7.36  75.41 19.41 22.49 25.45 28.06 32.31 35.53
      40.59
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H7OJ(16)        -0.43 85.56 24.15 29.0  33.26 36.92 43.23 47.77
      53.44 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC3H7OH           -60.69      76.31 20.87 25.94 30.62 34.65 41.04
      45.85 53.48
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C3H7O-N1=unknown1(1)      1.8100000e+13      0.00000
0.0000000e+00
!     CH2CHO+C2H5O-1=unknown1(1)    1.1500000e+13      0.00000
0.0000000e+00
!     C3H5OJ(13)+CH2OH=unknown1(1)  1.1500000e+13      0.00000
0.0000000e+00
!     C4H7OJ(16)+OH=unknown1(1)     7.7000000e+13      0.00000
0.0000000e+00
!     CO+nC3H7OH=unknown1(1)        9.1400000e+04      2.53000
8.5500000e+04

HCO+C3H7O-N1(+m)=CO+nC3H7OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -86.2309341262939
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8677000e+00 -1.3525000e+00 -4.5845000e-02 /
CHEB / 4.0682000e+00 1.0339000e+00 -4.0363000e-02 /
CHEB / 4.0412000e-01 4.8453000e-01 4.1793000e-02 /
CHEB / -2.2861000e-01 4.7386000e-02 6.0347000e-02 /
CHEB / -1.6188000e-01 -1.1457000e-01 2.1722000e-02 /

CH2CHO+C2H5O-1(+m)=HCO+C3H7O-N1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = 0.14983944540854743
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8423000e+00 -1.3525000e+00 -4.5845000e-02 /
CHEB / 3.2143000e+00 1.0339000e+00 -4.0363000e-02 /
CHEB / 1.4871000e-01 4.8453000e-01 4.1793000e-02 /
CHEB / -3.2397000e-01 4.7386000e-02 6.0347000e-02 /
CHEB / -1.9957000e-01 -1.1457000e-01 2.1722000e-02 /
```

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CH2CHO+C2H5O-1(+m)=CO+nC3H7OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -86.08109468088536
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6708000e+00 -1.3561000e+00 -4.5286000e-02 /
CHEB / 4.0864000e+00 1.0310000e+00 -4.0449000e-02 /
CHEB / 4.0161000e-01 4.8782000e-01 4.0597000e-02 /
CHEB / -2.3891000e-01 5.1651000e-02 5.9959000e-02 /
CHEB / -1.6766000e-01 -1.1319000e-01 2.2429000e-02 /

C3H5OJ(13)+CH2OH(+m)=HCO+C3H7O-N1(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
4.4094776060172105 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0430000e+01 -1.3172000e+00 -5.2145000e-02 /
CHEB / 2.5392000e+00 1.0590000e+00 -3.8730000e-02 /
CHEB / 1.5006000e-01 4.4906000e-01 5.4192000e-02 /
CHEB / -2.7087000e-01 8.0480000e-03 6.2883000e-02 /
CHEB / -1.6543000e-01 -1.2393000e-01 1.4084000e-02 /

C3H5OJ(13)+CH2OH(+m)=CH2CHO+C2H5O-1(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
4.55931705142576 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9119000e+00 -1.3205000e+00 -5.1608000e-02 /
CHEB / 2.5489000e+00 1.0567000e+00 -3.8949000e-02 /
CHEB / 1.6459000e-01 4.5251000e-01 5.3079000e-02 /
CHEB / -2.6637000e-01 1.1739000e-02 6.2763000e-02 /
CHEB / -1.6507000e-01 -1.2316000e-01 1.4853000e-02 /

C3H5OJ(13)+CH2OH(+m)=CO+nC3H7OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -90.64041173231112
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2423000e+00 -1.3205000e+00 -5.1608000e-02 /
CHEB / 3.4316000e+00 1.0567000e+00 -3.8949000e-02 /
CHEB / 3.9659000e-01 4.5251000e-01 5.3079000e-02 /
CHEB / -1.8509000e-01 1.1739000e-02 6.2763000e-02 /
CHEB / -1.3307000e-01 -1.2316000e-01 1.4853000e-02 /

C4H7OJ(16)+OH(+m)=HCO+C3H7O-N1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -9.148900761350026
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1830000e+01 -1.2760000e+00 -6.1556000e-02 /
CHEB / 1.9487000e+00 1.0778000e+00 -3.4073000e-02 /
CHEB / 1.3372000e-01 4.0470000e-01 6.8792000e-02 /
CHEB / -2.1730000e-01 -2.7758000e-02 6.2464000e-02 /
CHEB / -1.3086000e-01 -1.2613000e-01 4.8384000e-03 /
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```
C4H7OJ(16)+OH(+m)=CH2CHO+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
9.298740206758573 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1299000e+01 -1.2792000e+00 -6.1057000e-02 /
CHEB / 1.9720000e+00 1.0761000e+00 -3.4448000e-02 /
CHEB / 1.4501000e-01 4.0814000e-01 6.7842000e-02 /
CHEB / -2.1281000e-01 -2.4725000e-02 6.2617000e-02 /
CHEB / -1.2997000e-01 -1.2584000e-01 5.5998000e-03 /

C4H7OJ(16)+OH(+m)=C3H5OJ(13)+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
4.739423155332815 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0792000e+01 -1.2476000e+00 -6.6653000e-02 /
CHEB / 2.5668000e+00 1.0904000e+00 -3.0098000e-02 /
CHEB / 2.3016000e-01 3.7282000e-01 7.7396000e-02 /
CHEB / -1.8454000e-01 -5.2385000e-02 6.0312000e-02 /
CHEB / -1.1070000e-01 -1.2644000e-01 -1.9635000e-03 /

C4H7OJ(16)+OH(+m)=CO+nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -95.37983488764394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6294000e+00 -1.2792000e+00 -6.1057000e-02 /
CHEB / 2.8548000e+00 1.0761000e+00 -3.4448000e-02 /
CHEB / 3.7700000e-01 4.0814000e-01 6.7842000e-02 /
CHEB / -1.3154000e-01 -2.4725000e-02 6.2617000e-02 /
CHEB / -9.7979000e-02 -1.2584000e-01 5.5998000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(385)         -73.4 98.1  33.33 40.08 45.79 50.2  57.6  62.98
      69.59 null
!     nSPC(447)         -37.64      89.34 27.54 33.25 38.23 42.04 48.77
      53.38 59.21 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(447)+OH=nSPC(385)        2.0000000e+13      0.00000
0.0000000e+00

nSPC(447)+OH(+m)=nSPC(385)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown2) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
44.445337543518576 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1481000e+01 6.3839000e-01 -3.4136000e-02 /
CHEB / -3.3527000e+00 1.0289000e+00 -2.4932000e-02 /
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CHEB / -2.5110000e+00 5.0858000e-01 3.8385000e-02 /
CHEB / -1.5678000e+00 7.9232000e-02 4.6402000e-02 /
CHEB / -8.4594000e-01 -1.1023000e-01 1.1423000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -59.9 91.68 30.06 36.54 42.74 47.61 55.13 60.92
      68.42 null
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     nC4H8O+OH=unknown3(3)         2.7411173e+10      0.56667
3.7888889e+03
!     O+C4H9O-4=unknown3(3)   1.0000000e+13      0.00000
0.0000000e+00

O+C4H9O-4(+m)=nC4H8O+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #13 (unknown3)    deltaHrxn(T=298K) = -77.24237526529097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2148000e+01 -1.5436000e-06 -1.0744000e-06 /
CHEB / 1.5345000e-01 1.1063000e-07 7.7007000e-08 /
CHEB / 2.7591000e-01 7.1932000e-07 5.0070000e-07 /
CHEB / 9.9965000e-02 4.3089000e-07 2.9993000e-07 /
CHEB / 2.0813000e-02 1.4642000e-07 1.0192000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(301)         -53.93      102.11      32.84 39.97 46.09 50.94
      58.78 64.89 72.26 null
!     nSPC(351)         -46.74      102.81      35.54 42.8  48.89 53.6
      60.98 66.55 72.87 null
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-2+O2=nSPC(301)    3.7700000e+12      0.00000
0.0000000e+00
!     nSPC(301)=nSPC(351)           9.1600000e+08      1.12000
1.5380000e+04

C4H9O-2+O2(+m)=nSPC(301)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (unknown4) High-P Limit: R_Recombination estimate:
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(Average:) C_rad/H/NonDeC     O2_birad          deltaHrxn(T=298K) = -
34.90625207513041 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8591000e+00 3.7570000e+00 -6.0116000e-01 /
CHEB / -1.0457000e+01 2.0035000e+00 6.3453000e-01 /
CHEB / -5.2540000e+00 -4.5118000e-01 3.9348000e-01 /
CHEB / -1.8269000e+00 -6.5237000e-01 -9.8922000e-03 /
CHEB / -3.9436000e-01 -1.0719000e-01 -9.6448000e-02 /

nSPC(301)(+m)=nSPC(351)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (unknown4) High-P Limit: intra_H_migration exact:
R5H_SSSS_OO(Cs/Cs)Cs     O_rad_out     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = 7.18887994085933 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1898000e+00 9.8672000e-01 -4.8972000e-02 /
CHEB / -2.3361000e+00 1.2338000e+00 4.3019000e-03 /
CHEB / -4.4252000e+00 4.3731000e-02 7.6743000e-02 /
CHEB / -1.6506000e+00 -3.4742000e-01 6.5050000e-03 /
CHEB / -3.6383000e-01 -4.5376000e-02 -5.1624000e-02 /

C4H9O-2+O2(+m)=nSPC(351)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (unknown4)    deltaHrxn(T=298K) = -27.71737213427108
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2164000e+01 -5.1262000e-01 -1.9370000e-01 /
CHEB / 2.2092000e-01 6.7231000e-01 2.2258000e-01 /
CHEB / -2.2937000e-01 -8.2273000e-02 2.6667000e-02 /
CHEB / -1.4922000e-01 -1.1015000e-01 -6.0268000e-02 /
CHEB / -4.5041000e-02 -7.2573000e-04 -1.7468000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -83.87      107.63      38.47 46.26 53.36 58.49
      66.34 72.39 79.91 null
!     nSPC(385)         -73.4 98.1  33.33 40.08 45.79 50.2  57.6  62.98
      69.59 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     nSPC(351)         -46.74      102.81      35.54 42.8  48.89 53.6
      60.98 66.55 72.87 null
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(385)+OH=unknown5(5)      2.7411173e+10      0.56667
3.7888889e+03
!     O+nSPC(351)=unknown5(5) 1.0000000e+13      0.00000
0.0000000e+00

O+nSPC(351)(+m)=nSPC(385)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #22 (unknown5)    deltaHrxn(T=298K) = -77.60216405742754
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1456000e+01 -1.7277000e-06 -1.2026000e-06 /
CHEB / 7.9616000e-01 4.7018000e-08 3.2728000e-08 /
CHEB / 3.3999000e-01 9.8908000e-07 6.8847000e-07 /
CHEB / 1.2028000e-01 6.2365000e-07 4.3411000e-07 /
CHEB / 2.4402000e-02 1.8670000e-07 1.2996000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -101.86     95.2  29.58 36.6  42.74 48.02 56.4
      62.56 68.04 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9O-1           -16.27      88.99 26.95 32.82 38.15 42.65 49.68
      54.93 63.28  !MRH
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!Here are the path reactions and their high-P limit kinetics:
!     OH+C4H9O-1=unknown6(6)        7.7000000e+13      0.00000
0.0000000e+00
!     CH2OH+C3H7O-N1=unknown6(6)    1.1500000e+13      0.00000
0.0000000e+00
!     C2H5O-1+C2H5O-1=unknown6(6)   1.1500000e+13      0.00000
0.0000000e+00

OH+C4H9O-1(+m)=CH2OH+C3H7O-N1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (unknown6)    deltaHrxn(T=298K) = -7.229215568857242
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0783000e+01 -1.3449000e+00 -4.4982000e-02 /
CHEB / 3.0173000e+00 1.0497000e+00 -3.9904000e-02 /
CHEB / 2.1810000e-01 4.9124000e-01 4.3192000e-02 /
CHEB / -3.2422000e-01 3.4514000e-02 6.4489000e-02 /
CHEB / -2.0382000e-01 -1.3614000e-01 2.3199000e-02 /

OH+C4H9O-1(+m)=C2H5O-1+C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (unknown6)    deltaHrxn(T=298K) = -3.99958973754293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0271000e+01 -1.3290000e+00 -4.7144000e-02 /
CHEB / 3.3794000e+00 1.0626000e+00 -3.9338000e-02 /
CHEB / 2.2949000e-01 4.7497000e-01 4.8405000e-02 /
CHEB / -3.1704000e-01 1.3459000e-02 6.5827000e-02 /
CHEB / -1.9094000e-01 -1.4200000e-01 1.9288000e-02 /
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C2H5O-1+C2H5O-1(+m)=CH2OH+C3H7O-N1(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #25 (unknown6)     deltaHrxn(T=298K) = -
3.229625831314312 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5334000e+00 -1.3642000e+00 -4.2025000e-02 /
CHEB / 3.4858000e+00 1.0334000e+00 -4.0152000e-02 /
CHEB / 2.3761000e-01 5.1004000e-01 3.6524000e-02 /
CHEB / -3.4863000e-01 6.0380000e-02 6.1892000e-02 /
CHEB / -2.2439000e-01 -1.2780000e-01 2.7445000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -106.23     94.59 30.08 37.28 43.69 48.76 57.05
      63.06 70.55 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2CH[OH]C2H5     -20.29      85.12 28.32 34.19 39.3  43.58 50.27
      55.31 63.42  !MRH
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     HOCHC2H5          -17.02      78.74 21.22 25.67 29.69 33.11 38.51
      42.57 49.06
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C3H6O-enol2             -28.93      72.64 21.54 25.01 28.2  31.01
      35.6  39.14 44.92
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!Here are the path reactions and their high-P limit kinetics:
!     OH+CH2CH[OH]C2H5=unknown1(1)  7.7000000e+13      0.00000
0.0000000e+00
!     CH2OH+HOCHC2H5=unknown1(1)    4.7900000e+14      -0.75000
0.0000000e+00
!     C4H9O-3+OH=unknown1(1)        1.4157154e+13      -0.15000
2.9166667e+02
!     C2H5OH+C2H4O=unknown1(1)      1.6297242e+02      2.92024
4.4628571e+04
!     C3H6O-enol2+CH3OH=unknown1(1)       1.6297242e+02      2.92024
4.4628571e+04

OH+CH2CH[OH]C2H5(+m)=CH2OH+HOCHC2H5(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
9.258676895098185 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0646000e+01 -1.2730000e+00 -7.1229000e-02 /
CHEB / 2.4236000e+00 1.0889000e+00 -4.3033000e-02 /
CHEB / 2.3527000e-01 4.0931000e-01 8.2344000e-02 /
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CHEB / -2.1255000e-01 -3.9651000e-02 8.2013000e-02 /
CHEB / -1.4452000e-01 -1.4024000e-01 7.9750000e-03 /

OH+CH2CH[OH]C2H5(+m)=C2H5OH+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
73.75185909269328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0429000e+01 -1.3154000e+00 -6.7826000e-02 /
CHEB / 2.2096000e+00 1.0608000e+00 -4.9370000e-02 /
CHEB / 2.5907000e-01 4.5843000e-01 7.0352000e-02 /
CHEB / -1.4997000e-01 1.1456000e-02 8.7742000e-02 /
CHEB / -1.3056000e-01 -1.3353000e-01 2.4335000e-02 /

OH+CH2CH[OH]C2H5(+m)=C3H6O-enol2+CH3OH(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (unknown1)     deltaHrxn(T=298K)
= -65.79295869035728 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2998000e+00 -1.3017000e+00 -6.8413000e-02 /
CHEB / 2.6797000e+00 1.0711000e+00 -4.7314000e-02 /
CHEB / 3.8869000e-01 4.4288000e-01 7.3850000e-02 /
CHEB / -1.2532000e-01 -6.8895000e-03 8.5863000e-02 /
CHEB / -1.1932000e-01 -1.3737000e-01 1.8866000e-02 /

CH2OH+HOCHC2H5(+m)=C2H5OH+C2H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -64.49318219759509
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5263000e+00 -1.3656000e+00 -5.6511000e-02 /
CHEB / 2.4423000e+00 1.0291000e+00 -5.3127000e-02 /
CHEB / 2.8472000e-01 5.1137000e-01 4.8708000e-02 /
CHEB / -2.2875000e-01 6.8263000e-02 8.3913000e-02 /
CHEB / -1.8825000e-01 -1.2295000e-01 4.0099000e-02 /

CH2OH+HOCHC2H5(+m)=C3H6O-enol2+CH3OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
56.5342817952591 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1970000e+00 -1.3482000e+00 -5.8364000e-02 /
CHEB / 3.1074000e+00 1.0441000e+00 -5.1911000e-02 /
CHEB / 4.0322000e-01 4.9403000e-01 5.4514000e-02 /
CHEB / -2.1502000e-01 4.3296000e-02 8.4973000e-02 /
CHEB / -1.7473000e-01 -1.3158000e-01 3.4616000e-02 /

C4H9O-3+OH(+m)=OH+CH2CH[OH]C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -1.7897909596425734
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8984000e+00 -1.2241000e+00 -8.0004000e-02 /
CHEB / 4.1406000e+00 1.1056000e+00 -3.3146000e-02 /
CHEB / 5.2009000e-01 3.5070000e-01 9.7465000e-02 /
CHEB / -1.0648000e-01 -7.8153000e-02 7.2759000e-02 /
CHEB / -9.5369000e-02 -1.3380000e-01 -8.2047000e-03 /
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C4H9O-3+OH(+m)=CH2OH+HOCHC2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -11.048467854740759
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6198000e+00 -1.2587000e+00 -7.4569000e-02 /
CHEB / 2.1846000e+00 1.0932000e+00 -4.0186000e-02 /
CHEB / 1.9130000e-01 3.9265000e-01 8.7478000e-02 /
CHEB / -2.0960000e-01 -5.0346000e-02 7.9932000e-02 /
CHEB / -1.4568000e-01 -1.3835000e-01 3.2472000e-03 /

C4H9O-3+OH(+m)=C2H5OH+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -75.54165005233585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2770000e+00 -1.2987000e+00 -7.2078000e-02 /
CHEB / 2.0963000e+00 1.0681000e+00 -4.6984000e-02 /
CHEB / 2.0574000e-01 4.3986000e-01 7.7409000e-02 /
CHEB / -1.5286000e-01 -3.8815000e-03 8.7292000e-02 /
CHEB / -1.3013000e-01 -1.3385000e-01 1.8695000e-02 /

C4H9O-3+OH(+m)=C3H6O-enol2+CH3OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
67.58274964999985 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1911000e+00 -1.2859000e+00 -7.2303000e-02 /
CHEB / 2.5273000e+00 1.0772000e+00 -4.4773000e-02 /
CHEB / 3.3492000e-01 4.2500000e-01 8.0191000e-02 /
CHEB / -1.2597000e-01 -2.0452000e-02 8.4760000e-02 /
CHEB / -1.1907000e-01 -1.3672000e-01 1.3499000e-02 /

C3H6O-enol2+CH3OH(+m)=C2H5OH+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
7.958900402335992 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3169000e+01 -1.4108000e+00 -4.8024000e-02 /
CHEB / 2.0457000e+01 9.8886000e-01 -5.2926000e-02 /
CHEB / 8.5963000e-01 5.5140000e-01 3.0326000e-02 /
CHEB / -1.3788000e-01 1.3100000e-01 7.3543000e-02 /
CHEB / -1.8859000e-01 -9.6494000e-02 4.9328000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -111.86     93.14 31.04 37.84 44.35 49.5  57.51
      63.72 72.01 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
```

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!     C2H4O             -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!Here are the path reactions and their high-P limit kinetics:
!     OH+C4H9O-4=unknown2(2)        1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4O+C2H5OH=unknown2(2)      1.6297242e+02      2.92024
4.4628571e+04

OH+C4H9O-4(+m)=C2H4O+C2H5OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (unknown2)     deltaHrxn(T=298K) = -70.91241420293447
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9287000e+00 -1.3787000e+00 -4.7817000e-02 /
CHEB / 2.2781000e+00 1.0141000e+00 -4.6697000e-02 /
CHEB / 2.5252000e-01 5.1601000e-01 3.7223000e-02 /
CHEB / -2.1118000e-01 8.4756000e-02 6.7276000e-02 /
CHEB / -1.6130000e-01 -1.0840000e-01 3.4520000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       22.85 90.72 26.1  31.75 36.96 41.2  48.13 53.04
      58.94 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H6-13=unknown3(3)       5.2000000e+11      0.00000
6.5600000e+03
!     C3H4O+C2H3=unknown3(3)  1.4902950e+02      3.00740
1.0170800e+04
!     CO+C4H7-14=unknown3(3)        4.0416992e+07      1.70125
8.2775000e+04

HCO+C4H6-13(+m)=CO+C4H7-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (unknown3)     deltaHrxn(T=298K) = -16.578401545307017
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3818000e+01 -1.2438000e-04 -1.1319000e-04 /
CHEB / 2.2806000e+01 2.6837000e-04 2.2642000e-04 /
CHEB / -7.4047000e-03 -1.0667000e-04 -8.7906000e-05 /
CHEB / -4.2551000e-02 -2.7834000e-05 -2.0755000e-05 /
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CHEB / -4.3145000e-02 3.5401000e-06 4.7345000e-06 /

C3H4O+C2H3(+m)=HCO+C4H6-13(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (unknown3)     deltaHrxn(T=298K) = -18.967965984104676
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4555000e+00 -1.7739000e-01 -1.1359000e-01 /
CHEB / 4.7445000e+00 2.1991000e-01 1.3586000e-01 /
CHEB / 2.5427000e-01 -1.5096000e-02 -1.9259000e-03 /
CHEB / 4.4217000e-02 -3.0205000e-02 -2.0271000e-02 /
CHEB / -5.3358000e-03 -5.0918000e-03 -5.7947000e-03 /

C3H4O+C2H3(+m)=CO+C4H7-14(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (unknown3)     deltaHrxn(T=298K) = -35.54636752941168
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.5202000e+00 -1.4630000e-02 -1.0230000e-02 /
CHEB / 1.8432000e+01 1.6438000e-02 1.1502000e-02 /
CHEB / 6.8313000e-01 1.3941000e-04 8.8005000e-05 /
CHEB / 2.0111000e-01 -1.5954000e-03 -1.1174000e-03 /
CHEB / 3.7484000e-02 -5.0630000e-04 -3.5196000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       9.29  86.07 26.07 32.0  37.08 41.35 48.49 53.46
      59.59 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H6-13=unknown4(4)       5.2000000e+11      0.00000
6.5600000e+03
!     CO+C4H7-24=unknown4(4)        4.0416992e+07      1.70125
8.2775000e+04

HCO+C4H6-13(+m)=CO+C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #50 (unknown4)    deltaHrxn(T=298K) = -30.686986320012053
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.2421000e+00 -2.3890000e-02 -1.9915000e-02 /
CHEB / 1.8016000e+01 3.0965000e-02 2.5722000e-02 /
CHEB / -3.5908000e-02 -3.6614000e-03 -2.9208000e-03 /
CHEB / -4.4187000e-02 -4.6234000e-03 -3.8680000e-03 /
CHEB / -3.0751000e-02 1.3329000e-04 7.2526000e-05 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -30.44      96.46 30.22 36.43 41.63 45.96 53.16
      58.17 64.36 null
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+C3H4O=unknown5(5)      2.4827386e+10      0.24400
9.0875000e+03
!     CO+C4H7OJ(12)=unknown5(5)     9.1400000e+04      2.53000
8.5500000e+04

CH2CHO+C3H4O(+m)=CO+C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #117 (unknown5)   deltaHrxn(T=298K) = -23.327757723354516
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4006000e+01 -5.2311000e-02 -4.2985000e-02 /
CHEB / 2.1678000e+01 6.8499000e-02 5.5547000e-02 /
CHEB / 1.0801000e-02 -8.8271000e-03 -6.0500000e-03 /
CHEB / -5.1301000e-02 -9.9760000e-03 -8.4825000e-03 /
CHEB / -4.3496000e-02 -1.1257000e-05 -3.1487000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -2.3  80.93 23.54 31.43 38.38 43.73 52.09 57.89
      67.85 null
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     CH2O        -26.22      52.16 8.44  9.33  10.38 11.42 13.25 14.69
      16.9
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C2H4=unknown6(6)        6.9200000e+10      0.00000
4.3720000e+04
!     CH2O+C4H6-13=unknown6(6)      6.9200000e+10      0.00000
4.3720000e+04

CH2O+C4H6-13(+m)=C3H4O+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #163 (unknown6)   deltaHrxn(T=298K) = -3.379718960028404
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.6558000e+00 -1.2883000e+00 -6.0206000e-02 /
CHEB / 1.6914000e+01 1.0766000e+00 -3.5343000e-02 /
CHEB / -8.0234000e-02 4.2796000e-01 6.9919000e-02 /
CHEB / -3.0142000e-01 -1.0710000e-02 6.8793000e-02 /
CHEB / -1.5064000e-01 -1.3144000e-01 8.4867000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -24.21      89.88 27.61 33.82 39.16 43.67 51.24
      56.6  63.44 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C3H5OJ(13)        7.36  75.41 19.41 22.49 25.45 28.06 32.31 35.53
      40.59
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H7-14=unknown7(7)       1.8100000e+13      0.00000
0.0000000e+00
!     CH2CHO+aC3H5=unknown7(7)      1.1500000e+13      0.00000
0.0000000e+00
!     C3H5OJ(13)+C2H3=unknown7(7)   1.4157154e+13      -0.15000
2.9166667e+02
!     CO+C4H8-1=unknown7(7)         9.1400000e+04      2.53000
8.5500000e+04

HCO+C4H7-14(+m)=CH2CHO+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (unknown7)   deltaHrxn(T=298K) = -12.178640665466489
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0761000e+01 -1.3700000e+00 -5.2104000e-02 /
CHEB / 2.1354000e+00 1.0148000e+00 -4.7835000e-02 /
CHEB / 1.7266000e-01 4.9812000e-01 4.2643000e-02 /
CHEB / -2.7229000e-01 7.3882000e-02 6.8572000e-02 /
CHEB / -1.8999000e-01 -1.0143000e-01 3.1105000e-02 /

HCO+C4H7-14(+m)=CO+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (unknown7)   deltaHrxn(T=298K) = -83.52155181906336
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8655000e+00 -1.2955000e+00 -6.4574000e-02 /
CHEB / 4.9683000e+00 1.0658000e+00 -4.1304000e-02 /
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CHEB / 5.5980000e-01 4.2468000e-01 6.8949000e-02 /
CHEB / -1.2496000e-01 -7.7333000e-03 7.1403000e-02 /
CHEB / -1.0347000e-01 -1.2227000e-01 1.2264000e-02 /

CH2CHO+aC3H5(+m)=CO+C4H8-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (unknown7)   deltaHrxn(T=298K) = -71.34291115359687
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2786000e+00 -1.3569000e+00 -5.4822000e-02 /
CHEB / 7.6814000e+00 1.0242000e+00 -4.7174000e-02 /
CHEB / 3.6291000e-01 4.8608000e-01 4.7737000e-02 /
CHEB / -1.9229000e-01 5.9507000e-02 7.0083000e-02 /
CHEB / -1.5164000e-01 -1.0589000e-01 2.8265000e-02 /

C3H5OJ(13)+C2H3(+m)=HCO+C4H7-14(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (unknown7)   deltaHrxn(T=298K) = -20.587655766469283
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1391000e+01 -1.0400000e+00 -1.4432000e-01 /
CHEB / 1.1621000e+00 1.0046000e+00 5.0981000e-02 /
CHEB / 1.6428000e-01 2.2198000e-01 1.1208000e-01 /
CHEB / -8.9641000e-02 -8.6665000e-02 3.2724000e-02 /
CHEB / -7.2307000e-02 -9.3202000e-02 -2.5348000e-02 /

C3H5OJ(13)+C2H3(+m)=CH2CHO+aC3H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (unknown7)    deltaHrxn(T=298K) = -
32.76629643193578 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1599000e+01 -1.0695000e+00 -1.4747000e-01 /
CHEB / 5.8790000e-01 9.9330000e-01 4.5117000e-02 /
CHEB / -3.3727000e-02 2.5906000e-01 1.1221000e-01 /
CHEB / -1.4096000e-01 -6.3932000e-02 4.2808000e-02 /
CHEB / -9.0621000e-02 -9.6115000e-02 -1.8901000e-02 /

C3H5OJ(13)+C2H3(+m)=CO+C4H8-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (unknown7)   deltaHrxn(T=298K) = -104.10920758553266
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7044000e+00 -1.0340000e+00 -1.4430000e-01 /
CHEB / 2.4065000e+00 1.0055000e+00 5.2351000e-02 /
CHEB / 4.9233000e-01 2.1502000e-01 1.1220000e-01 /
CHEB / 2.1188000e-02 -8.9972000e-02 3.0960000e-02 /
CHEB / -2.8843000e-02 -9.2172000e-02 -2.6343000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -26.15      87.01 26.64 33.01 38.88 43.66 51.4
      56.88 62.78 null
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!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H7-24=unknown1(1)       1.4157154e+13      -0.15000
2.9166667e+02
!     CO+C4H8-1=unknown1(1)         7.6600000e+05      2.07000
8.2200000e+04

HCO+C4H7-24(+m)=CO+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -69.41296704435833
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5194000e+00 -1.2604000e+00 -7.1361000e-02 /
CHEB / 6.8877000e+00 1.0764000e+00 -3.3131000e-02 /
CHEB / 3.6990000e-01 3.8949000e-01 7.8405000e-02 /
CHEB / -1.1756000e-01 -3.2128000e-02 6.6635000e-02 /
CHEB / -9.8408000e-02 -1.2277000e-01 3.9210000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -25.92      85.38 26.29 32.88 38.76 43.79 51.68
      57.48 62.63 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H7-24=unknown2(2)       1.4157154e+13      -0.15000
2.9166667e+02
!     CO+C4H8-2=unknown2(2)         9.1400000e+04      2.53000
8.5500000e+04

HCO+C4H7-24(+m)=CO+C4H8-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8 (unknown2)     deltaHrxn(T=298K) = -72.13277022982838
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4824000e+00 -1.2159000e+00 -7.9925000e-02 /
CHEB / 7.0592000e+00 1.0826000e+00 -2.0662000e-02 /
CHEB / 3.6278000e-01 3.4475000e-01 8.7185000e-02 /
CHEB / -1.0263000e-01 -5.8702000e-02 5.8016000e-02 /
CHEB / -9.1484000e-02 -1.1993000e-01 -5.7392000e-03 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -75.23      95.38 30.29 36.53 42.46 47.55 55.8
      61.56 67.4  null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H7OJ(12)=unknown3(3)    1.4157154e+13      -0.15000
2.9166667e+02
!     CO+nC4H8O=unknown3(3)         7.6600000e+05      2.07000
8.2200000e+04

HCO+C4H7OJ(12)(+m)=CO+nC4H8O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #23 (unknown3)    deltaHrxn(T=298K) = -79.60214495416432
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5221000e+00 -1.4229000e+00 -4.0761000e-02 /
CHEB / 5.5023000e+00 9.6880000e-01 -4.5776000e-02 /
CHEB / 4.7029000e-01 5.4347000e-01 2.2401000e-02 /
CHEB / -3.0947000e-01 1.4028000e-01 5.6760000e-02 /
CHEB / -2.4638000e-01 -7.4903000e-02 3.8915000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       -37.09      107.53      32.16 41.48 48.19 53.65
      62.39 68.65 75.41 null
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+aC3H5O2=unknown4(4)    1.4157154e+13      -0.15000
2.9166667e+02
!     nSPC(543)+aC3H5=unknown4(4)   1.4157154e+13      -0.15000
2.9166667e+02

CH2CHO+aC3H5O2(+m)=nSPC(543)+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #34 (unknown4)     deltaHrxn(T=298K) = -
4.8895982280706605 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1576000e+00 -6.6845000e-01 -1.8746000e-01 /
CHEB / 2.5038000e+00 7.7068000e-01 1.6922000e-01 /
CHEB / 4.0869000e-01 1.0406000e-02 6.6757000e-02 /
CHEB / -2.3319000e-03 -9.9569000e-02 -2.6336000e-02 /
CHEB / -2.3417000e-02 -3.4262000e-02 -2.7633000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -82.61      119.61      39.97 51.05 58.73 64.73
      73.75 79.91 87.49 null
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(801)+aC3H5O2=unknown5(5) 1.4157154e+13      -0.15000
2.9166667e+02
!     nSPC(879)+aC3H5=unknown5(5)   1.4157154e+13      -0.15000
2.9166667e+02

nSPC(801)+aC3H5O2(+m)=nSPC(879)+aC3H5(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #61 (unknown5)     deltaHrxn(T=298K) = -
12.878244734748357 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1830000e+00 -5.9148000e-01 -1.7747000e-01 /
CHEB / 2.6315000e+00 7.3205000e-01 1.8219000e-01 /
CHEB / 3.8625000e-01 -5.0713000e-02 4.3598000e-02 /
CHEB / 4.3595000e-03 -1.0143000e-01 -3.9391000e-02 /
CHEB / 9.8819000e-04 -1.2802000e-02 -2.1184000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       41.97 84.06 25.26 31.72 37.54 42.31 49.95 55.61
      65.41 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C3H6=unknown6(6)   1.4902950e+02      3.00740
1.0170800e+04
```

```
!     C4H6-13+CH3=unknown6(6)       2.4300000e+12      0.00000
1.0200000e+04

C2H3+C3H6(+m)=C4H6-13+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #116 (unknown6)   deltaHrxn(T=298K) = -14.238824258588558
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0169000e+00 -7.8940000e-01 -1.9036000e-01 /
CHEB / 5.2437000e+00 8.6278000e-01 1.4647000e-01 /
CHEB / 2.7396000e-01 7.6397000e-02 9.4073000e-02 /
CHEB / -1.2479000e-02 -1.1119000e-01 -1.2380000e-02 /
CHEB / -2.3561000e-02 -6.1199000e-02 -3.6258000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       11.15 84.52 26.03 33.97 41.4  46.77 55.52 61.64
      75.21 null
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+C3H6=unknown1(1)       6.9200000e+10      0.00000
4.3720000e+04
!     CH3CHO+aC3H5=unknown1(1)      6.9200000e+10      0.00000
4.3720000e+04

CH2CHO+C3H6(+m)=CH3CHO+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -8.189142750404748
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8774000e+00 -7.7995000e-01 -1.7290000e-01 /
CHEB / 1.5481000e+01 8.7154000e-01 1.3719000e-01 /
CHEB / -4.9604000e-02 5.4655000e-02 8.2893000e-02 /
CHEB / -1.0295000e-01 -1.1833000e-01 -1.5607000e-02 /
CHEB / -3.3639000e-02 -5.4575000e-02 -3.2938000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -5.51 88.37 29.57 37.77 44.37 49.58 57.38 63.22
      69.88 null
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
```

```
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C2H5=unknown2(2)        2.3501400e+11      0.30815
4.9629937e+03
!     C3H5O-enol2+C2H4=unknown2(2)  1.1691492e+02      2.87714
4.8857143e+04

C3H4O+C2H5(+m)=C3H5O-enol2+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #12 (unknown2)    deltaHrxn(T=298K) = -3.059602893916489
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0155000e+00 1.0282000e-07 7.0497000e-08 /
CHEB / 1.6775000e+01 2.0325000e-07 1.4177000e-07 /
CHEB / 3.4870000e-01 1.6816000e-07 1.1840000e-07 /
CHEB / 1.1120000e-01 1.1221000e-07 7.8105000e-08 /
CHEB / 2.3938000e-02 6.7247000e-08 4.6098000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -7.13 92.79 28.53 35.15 41.29 46.34 54.5  60.43
      67.96 null
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C2H5=unknown3(3)        7.2517543e+09      0.48800
1.0375000e+04
!     C4H8-1+HCO=unknown3(3)        5.2000000e+11      0.00000
6.5600000e+03

C3H4O+C2H5(+m)=C4H8-1+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #33 (unknown3)    deltaHrxn(T=298K) = -3.2696763081174467
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7655000e+00 -4.0131000e-01 -1.7031000e-01 /
CHEB / 3.9274000e+00 4.8452000e-01 1.9066000e-01 /
CHEB / -1.3346000e-02 -1.5488000e-02 1.4781000e-02 /
CHEB / -5.8961000e-02 -6.9148000e-02 -2.9164000e-02 /
CHEB / -3.2010000e-02 -1.6711000e-02 -1.4512000e-02 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       8.14  86.58 25.68 33.73 40.93 46.4  55.15 61.29
      71.69 null
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+C2H4O=unknown4(4) 6.9200000e+10      0.00000
4.3720000e+04
!     C3H5O-enol2+C2H4=unknown4(4)  6.9200000e+10      0.00000
4.3720000e+04

aC3H5+C2H4O(+m)=C3H5O-enol2+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #47 (unknown4)     deltaHrxn(T=298K) = -
0.7497931910405953 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0922000e+01 -9.3191000e-01 -1.7541000e-01 /
CHEB / 1.7424000e+01 9.4179000e-01 8.9376000e-02 /
CHEB / 1.3036000e-01 1.5063000e-01 1.2144000e-01 /
CHEB / -1.8455000e-01 -8.1609000e-02 1.7548000e-02 /
CHEB / -1.2689000e-01 -7.4413000e-02 -3.1538000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -7.68 91.08 28.3  35.55 41.68 46.82 54.83 60.63
      67.46 null
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     C4H6-13+CH2OH=unknown5(5)     2.4100000e+10      0.00000
6.9600000e+03
!     C3H5O-enol2+C2H4=unknown5(5)  1.6297242e+02      2.92024
4.4628571e+04

C4H6-13+CH2OH(+m)=C3H5O-enol2+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #84 (unknown5)     deltaHrxn(T=298K) = -
12.938574079791993 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5011000e+00 -1.0495000e+00 -1.4684000e-01 /
CHEB / 1.2140000e+01 1.0254000e+00 4.5123000e-02 /
CHEB / 9.8529000e-02 2.2738000e-01 1.2620000e-01 /
CHEB / -1.1627000e-01 -9.5371000e-02 3.9570000e-02 /
CHEB / -8.2979000e-02 -1.0429000e-01 -3.1306000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       6.17  94.7  28.36 35.23 41.26 46.18 54.06 59.78
      67.6  null
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol2+C2H3=unknown6(6)  1.4902950e+02      3.00740
1.0170800e+04
!     C4H6-13+CH2OH=unknown6(6)     7.2517543e+09      0.48800
1.0375000e+04

C3H6O-enol2+C2H3(+m)=C4H6-13+CH2OH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #134 (unknown6)    deltaHrxn(T=298K) = -
18.157772162707847 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5558000e+00 -9.7281000e-01 -1.5476000e-01 /
CHEB / 5.5653000e+00 1.0161000e+00 6.8456000e-02 /
CHEB / 2.0983000e-01 1.4786000e-01 1.2711000e-01 /
CHEB / -7.3313000e-02 -1.2107000e-01 1.6360000e-02 /
CHEB / -7.1513000e-02 -8.8379000e-02 -4.1005000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -43.81      106.65      32.02 38.49 44.04 49.15
      57.82 63.57 69.34 null
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
```

```
!     C3H6O-enol2+CH2CHO=unknown7(7)      2.4827386e+10      0.24400
9.0875000e+03
!     C4H9O-3+CO=unknown7(7)        9.1400000e+04      2.53000
8.5500000e+04

C3H6O-enol2+CH2CHO(+m)=C4H9O-3+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #195 (unknown7)    deltaHrxn(T=298K) = -
20.758089958702787 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5203000e+01 -8.6848000e-02 -6.5652000e-02 /
CHEB / 2.2907000e+01 1.1472000e-01 8.4995000e-02 /
CHEB / 1.4001000e-01 -1.7610000e-02 -1.0112000e-02 /
CHEB / 3.4022000e-03 -1.4360000e-02 -1.2108000e-02 /
CHEB / -2.8301000e-02 3.8687000e-04 -3.7801000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown8(8)       -41.31      99.01 32.67 41.28 48.09 53.45 61.49
      67.39 72.07 null
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C2H5O-1=unknown8(8)     2.3501400e+11      0.30815
4.9629937e+03
!     C3H5O-enol2+C2H4O=unknown8(8) 1.1691492e+02      2.87714
4.8857143e+04

C3H4O+C2H5O-1(+m)=C3H5O-enol2+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #276 (unknown8)    deltaHrxn(T=298K) = -
10.508855203322582 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.9673000e+00 -2.4504000e-03 -2.0669000e-03 /
CHEB / 1.4329000e+01 3.3459000e-03 2.8222000e-03 /
CHEB / 3.8144000e-01 -6.0468000e-04 -5.1020000e-04 /
CHEB / 1.1264000e-01 -5.5652000e-04 -4.6875000e-04 /
CHEB / 1.5299000e-02 2.0157000e-04 1.6946000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown10(10)     -42.83      90.99 28.9  36.49 43.18 48.64 57.33
      63.62 71.44 null
```

```
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C4H7-24+CH2OH=unknown10(10)   4.7900000e+14      -0.75000
0.0000000e+00
!     C4H6-13+CH3OH=unknown10(10)   1.6297242e+02      2.92024
4.4628571e+04
!     C2H4O+C3H6=unknown10(10)      1.6297242e+02      2.92024
4.4628571e+04

C4H7-24+CH2OH(+m)=C4H6-13+CH3OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #375 (unknown10)  deltaHrxn(T=298K) = -50.454546134635336
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0295000e+00 -1.4216000e+00 -4.0816000e-02 /
CHEB / 4.2971000e+00 9.7821000e-01 -4.6507000e-02 /
CHEB / 5.2650000e-01 5.6029000e-01 2.2786000e-02 /
CHEB / -2.6782000e-01 1.4813000e-01 6.1067000e-02 /
CHEB / -2.2700000e-01 -8.6836000e-02 4.3728000e-02 /

C4H7-24+CH2OH(+m)=C2H4O+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #375 (unknown10)  deltaHrxn(T=298K) = -53.81442522315771
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4665000e+00 -1.4299000e+00 -3.9797000e-02 /
CHEB / 3.8178000e+00 9.6941000e-01 -4.6400000e-02 /
CHEB / 4.6639000e-01 5.6629000e-01 2.0078000e-02 /
CHEB / -2.8316000e-01 1.6096000e-01 5.8808000e-02 /
CHEB / -2.4111000e-01 -7.9209000e-02 4.4537000e-02 /

C4H6-13+CH3OH(+m)=C2H4O+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #375 (unknown10)  deltaHrxn(T=298K) = -3.3598790885223826
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3703000e+01 -1.4504000e+00 -3.7195000e-02 /
CHEB / 2.1389000e+01 9.4676000e-01 -4.5902000e-02 /
CHEB / 9.4958000e-01 5.7902000e-01 1.3350000e-02 /
CHEB / -1.6950000e-01 1.9175000e-01 5.2465000e-02 /
CHEB / -2.1119000e-01 -5.8798000e-02 4.5656000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -21.35      99.27 32.66 41.53 49.43 55.22 64.52
      71.38 83.77 null
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     aC3H5O2           24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67
      46.07
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!Here are the path reactions and their high-P limit kinetics:
!     CH3CHO+aC3H5O2=unknown1(1)    6.9200000e+10      0.00000
4.3720000e+04
!     C3H6+nSPC(543)=unknown1(1)    6.9200000e+10      0.00000
4.3720000e+04

C3H6+nSPC(543)(+m)=CH3CHO+aC3H5O2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
3.299544522334081 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0398000e+01 -5.1911000e-01 -1.8544000e-01 /
CHEB / 1.7106000e+01 6.3788000e-01 1.9791000e-01 /
CHEB / 2.7801000e-01 -3.9468000e-02 3.2172000e-02 /
CHEB / -1.4668000e-02 -8.7098000e-02 -3.6814000e-02 /
CHEB / -1.6333000e-02 -1.2278000e-02 -1.8877000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -38.67      90.96 30.44 38.77 45.7  51.26 59.69
      66.07 73.61 null
!     CH2CHO      6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34 26.35
Neither TRange included 298K!
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+C3H7-1=unknown2(2)     1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4O+C3H6=unknown2(2)  1.1691492e+02      2.87714
4.8857143e+04

CH2CHO+C3H7-1(+m)=C2H4O+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (unknown2)     deltaHrxn(T=298K) = -54.081469956407624
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2180000e+00 -1.4148000e+00 -5.3036000e-02 /
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CHEB / 3.2105000e+00 9.5085000e-01 -5.8795000e-02 /
CHEB / -2.7209000e-01 4.7903000e-01 2.4407000e-02 /
CHEB / -7.7693000e-01 8.8321000e-02 5.7856000e-02 /
CHEB / -5.3446000e-01 -7.0486000e-02 3.4969000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -40.84      93.67 29.17 36.55 43.01 48.5  57.14
      63.48 71.19 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C3H7O-N1=unknown3(3)     1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+C2H5O-1=unknown3(3)     1.1500000e+13      0.00000
0.0000000e+00
!     C3H6O-enol2+C2H4=unknown3(3)  1.6297242e+02      2.92024
4.4628571e+04

C2H3+C3H7O-N1(+m)=aC3H5+C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (unknown3)     deltaHrxn(T=298K) = -24.977353549195698
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0916000e+01 -1.2731000e+00 -7.0488000e-02 /
CHEB / 1.5054000e+00 1.0748000e+00 -3.5644000e-02 /
CHEB / 7.6910000e-02 4.1004000e-01 7.7098000e-02 /
CHEB / -2.0643000e-01 -2.3850000e-02 7.1858000e-02 /
CHEB / -1.3554000e-01 -1.3098000e-01 7.5252000e-03 /

C2H3+C3H7O-N1(+m)=C3H6O-enol2+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (unknown3)      deltaHrxn(T=298K) = -
76.60219913808947 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2053000e+00 -1.2903000e+00 -6.8789000e-02 /
CHEB / 2.1727000e+00 1.0640000e+00 -3.8145000e-02 /
CHEB / 2.3353000e-01 4.2899000e-01 7.2416000e-02 /
CHEB / -1.4286000e-01 -4.2296000e-03 7.3498000e-02 /
CHEB / -1.1252000e-01 -1.2751000e-01 1.2847000e-02 /

aC3H5+C2H5O-1(+m)=C3H6O-enol2+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (unknown3)      deltaHrxn(T=298K) = -
51.624845588893784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

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CHEB / 5    3 /
CHEB / 6.5899000e+00 -1.4568000e+00 -3.5453000e-02 /
CHEB / 4.3574000e+00 9.3370000e-01 -4.3865000e-02 /
CHEB / 5.6419000e-01 5.6838000e-01 1.1816000e-02 /
CHEB / -2.8771000e-01 1.9035000e-01 4.7852000e-02 /
CHEB / -2.6085000e-01 -4.7008000e-02 4.1820000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       -44.18      91.2  29.72 37.5  44.24 49.54 58.07
      64.24 73.1  null
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!Here are the path reactions and their high-P limit kinetics:
!     C3H5O-enol2+C2H5=unknown4(4)  4.7900000e+14      -0.75000
0.0000000e+00
!     C4H6-13+CH3OH=unknown4(4)     1.6297242e+02      2.92024
4.4628571e+04

C3H5O-enol2+C2H5(+m)=C4H6-13+CH3OH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #24 (unknown4)     deltaHrxn(T=298K) = -
47.56491002015005 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3728000e+00 -1.4490000e+00 -4.2880000e-02 /
CHEB / 4.7907000e+00 9.4308000e-01 -5.2450000e-02 /
CHEB / 5.6656000e-01 5.6631000e-01 1.5392000e-02 /
CHEB / -2.9087000e-01 1.8227000e-01 5.8144000e-02 /
CHEB / -2.6469000e-01 -5.3958000e-02 4.9645000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -35.72      80.41 26.03 34.59 42.43 48.57 58.22
      65.02 77.61 null
!     CH2O        -26.22      52.16 8.44  9.33  10.38 11.42 13.25 14.69
      16.9
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
```

```
!     CH2O+C4H8-2=unknown5(5) 6.9200000e+10      0.00000
4.3720000e+04
!     CH3CHO+C3H6=unknown5(5)       2.3300000e+06      1.65000
5.4150000e+04

CH2O+C4H8-2(+m)=CH3CHO+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #47 (unknown5)    deltaHrxn(T=298K) = -5.939179978655356
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0450000e+01 -1.2470000e+00 -5.7042000e-02 /
CHEB / 1.8676000e+01 1.1041000e+00 -2.5564000e-02 /
CHEB / -3.9630000e-02 3.8128000e-01 7.1712000e-02 /
CHEB / -2.9566000e-01 -6.1392000e-02 5.5017000e-02 /
CHEB / -9.9330000e-02 -1.4155000e-01 -5.2049000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -74.47      101.6 33.54 42.28 49.42 55.13 63.8
      70.24 75.8  null
!     CH2CHO      6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34 26.35
Neither TRange included 298K!
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+C3H7O-N1=unknown6(6)   1.4157154e+13      -0.15000
2.9166667e+02
!     C2H4O+C3H6O-enol2=unknown6(6) 1.1691492e+02      2.87714
4.8857143e+04

CH2CHO+C3H7O-N1(+m)=C2H4O+C3H6O-enol2(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #50 (unknown6)     deltaHrxn(T=298K) = -
53.07181291613155 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7973000e+00 -1.3860000e+00 -4.0444000e-02 /
CHEB / 4.7467000e+00 1.0108000e+00 -4.0991000e-02 /
CHEB / 4.6319000e-01 5.2638000e-01 3.0768000e-02 /
CHEB / -2.8639000e-01 9.4576000e-02 5.8478000e-02 /
CHEB / -2.1428000e-01 -1.0751000e-01 3.0588000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -93.06      99.94 32.99 40.93 47.99 53.57 62.62
      69.06 76.74 null
```

```
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H9O-4=unknown7(7)       1.4157154e+13      -0.15000
2.9166667e+02
!     CO+nC4H10O=unknown7(7)        7.6600000e+05      2.07000
8.2200000e+04
!     C3H4O+C2H5OH=unknown7(7)      1.6297242e+02      2.92024
4.4628571e+04

HCO+C4H9O-4(+m)=CO+nC4H10O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #84 (unknown7)    deltaHrxn(T=298K) = -79.4719432157442
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3346000e+00 -1.3150000e+00 -6.4719000e-02 /
CHEB / 4.7733000e+00 1.0637000e+00 -4.8868000e-02 /
CHEB / 4.5351000e-01 4.5477000e-01 6.7583000e-02 /
CHEB / -1.9086000e-01 5.4966000e-03 8.4305000e-02 /
CHEB / -1.5557000e-01 -1.3384000e-01 2.2314000e-02 /

HCO+C4H9O-4(+m)=C3H4O+C2H5OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #84 (unknown7)    deltaHrxn(T=298K) = -57.383874279810286
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4940000e+00 -1.3651000e+00 -5.7667000e-02 /
CHEB / 2.9299000e+00 1.0267000e+00 -5.3578000e-02 /
CHEB / 3.6593000e-01 5.0698000e-01 4.9360000e-02 /
CHEB / -2.1314000e-01 6.8099000e-02 8.3253000e-02 /
CHEB / -1.8991000e-01 -1.1843000e-01 3.9089000e-02 /

!C3H4O+C2H5OH(+m)=CO+nC4H10O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #84 (unknown7)    deltaHrxn(T=298K) = -22.08806893593392
kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / -1.7726000e+01 -1.3535000e+00 -6.0085000e-02 /
!CHEB / 2.4091000e+01 1.0350000e+00 -5.2887000e-02 /
!CHEB / 5.8938000e-01 4.9529000e-01 5.4323000e-02 /
!CHEB / -1.3407000e-01 5.4061000e-02 8.4557000e-02 /
!CHEB / -1.5678000e-01 -1.2213000e-01 3.5651000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     unknown8(8)       -90.16      102.21      33.52 40.82 47.14 52.54
      61.57 68.02 74.54 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H9O-1           -16.27      88.99 26.95 32.82 38.15 42.65 49.68
      54.93 63.28  !MRH
!     CH2CHO      6.0   64.0  13.18 15.15 16.96 18.6  21.3  23.34 26.35
Neither TRange included 298K!
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H9O-1=unknown8(8)       1.8100000e+13      0.00000
0.0000000e+00
!     CH2CHO+C3H7O-N1=unknown8(8)   1.1500000e+13      0.00000
0.0000000e+00
!     CO+nC4H10O=unknown8(8)        9.1400000e+04      2.53000
8.5500000e+04

HCO+C4H9O-1(+m)=CO+nC4H10O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #112 (unknown8)   deltaHrxn(T=298K) = -86.33118189108755
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2887000e+00 -1.4218000e+00 -3.4879000e-02 /
CHEB / 5.6839000e+00 9.7839000e-01 -4.0034000e-02 /
CHEB / 5.9379000e-01 5.6014000e-01 1.8991000e-02 /
CHEB / -3.3244000e-01 1.4570000e-01 5.2010000e-02 /
CHEB / -2.6220000e-01 -8.9513000e-02 3.7526000e-02 /

CH2CHO+C3H7O-N1(+m)=HCO+C4H9O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #112 (unknown8)   deltaHrxn(T=298K) = -1.2168555005370383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3831000e+00 -1.4149000e+00 -3.5588000e-02 /
CHEB / 4.4989000e+00 9.8595000e-01 -4.0079000e-02 /
CHEB / 3.1539000e-01 5.5582000e-01 2.0949000e-02 /
CHEB / -4.2091000e-01 1.3555000e-01 5.3603000e-02 /
CHEB / -2.9064000e-01 -9.6026000e-02 3.6868000e-02 /

CH2CHO+C3H7O-N1(+m)=CO+nC4H10O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #112 (unknown8)   deltaHrxn(T=298K) = -87.54803739162459
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2954000e+00 -1.4171000e+00 -3.5359000e-02 /
CHEB / 5.4662000e+00 9.8351000e-01 -4.0068000e-02 /
CHEB / 5.9466000e-01 5.5725000e-01 2.0310000e-02 /
CHEB / -3.2488000e-01 1.3886000e-01 5.3093000e-02 /
CHEB / -2.5501000e-01 -9.3933000e-02 3.7094000e-02 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown9(9)       -91.93      99.72 32.17 39.92 46.93 52.67 61.88
      68.44 73.99 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H9O-3=unknown9(9)       1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7OJ(12)+CH2OH=unknown9(9)  4.7900000e+14      -0.75000
0.0000000e+00
!     CO+nC4H10O=unknown9(9)        7.6600000e+05      2.07000
8.2200000e+04
!     C3H4O+C2H5OH=unknown9(9)      1.6297242e+02      2.92024
4.4628571e+04

HCO+C4H9O-3(+m)=C4H7OJ(12)+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #142 (unknown9)    deltaHrxn(T=298K) = -
1.759473943254902 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3462000e+00 -1.3857000e+00 -4.5331000e-02 /
CHEB / 4.0835000e+00 1.0181000e+00 -4.7137000e-02 /
CHEB / 2.0666000e-01 5.3849000e-01 3.4993000e-02 /
CHEB / -4.0228000e-01 9.3546000e-02 7.2805000e-02 /
CHEB / -2.7205000e-01 -1.2444000e-01 4.2177000e-02 /

HCO+C4H9O-3(+m)=CO+nC4H10O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #142 (unknown9)   deltaHrxn(T=298K) = -84.10117906514557
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2561000e+00 -1.3840000e+00 -4.5524000e-02 /
CHEB / 5.2310000e+00 1.0197000e+00 -4.7118000e-02 /
CHEB / 4.8575000e-01 5.3698000e-01 3.5508000e-02 /
CHEB / -3.0365000e-01 9.0946000e-02 7.3067000e-02 /
CHEB / -2.3167000e-01 -1.2561000e-01 4.1825000e-02 /

HCO+C4H9O-3(+m)=C3H4O+C2H5OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #142 (unknown9)   deltaHrxn(T=298K) = -62.013110129211654
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2010000e+00 -1.4168000e+00 -4.1835000e-02 /
CHEB / 3.5918000e+00 9.8704000e-01 -4.6967000e-02 /
CHEB / 3.7204000e-01 5.6500000e-01 2.6010000e-02 /
CHEB / -3.1626000e-01 1.4399000e-01 6.6900000e-02 /
CHEB / -2.7138000e-01 -9.8224000e-02 4.6958000e-02 /

C4H7OJ(12)+CH2OH(+m)=CO+nC4H10O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #142 (unknown9)   deltaHrxn(T=298K) = -82.34170512189067
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9945000e+00 -1.3929000e+00 -4.4451000e-02 /
CHEB / 5.1441000e+00 1.0112000e+00 -4.7156000e-02 /
CHEB / 4.1145000e-01 5.4482000e-01 3.2733000e-02 /
CHEB / -3.5424000e-01 1.0469000e-01 7.1526000e-02 /
CHEB / -2.5656000e-01 -1.1923000e-01 4.3570000e-02 /

C4H7OJ(12)+CH2OH(+m)=C3H4O+C2H5OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #142 (unknown9)    deltaHrxn(T=298K) = -
60.25363618595676 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1206000e+00 -1.4264000e+00 -4.0454000e-02 /
CHEB / 3.2944000e+00 9.7687000e-01 -4.6564000e-02 /
CHEB / 3.4375000e-01 5.7194000e-01 2.2895000e-02 /
CHEB / -3.6448000e-01 1.5912000e-01 6.4040000e-02 /
CHEB / -2.9834000e-01 -8.9019000e-02 4.7581000e-02 /

C3H4O+C2H5OH(+m)=CO+nC4H10O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #142 (unknown9)   deltaHrxn(T=298K) = -22.08806893593392
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8427000e+01 -1.4246000e+00 -4.0718000e-02 /
CHEB / 2.5170000e+01 9.7885000e-01 -4.6648000e-02 /
CHEB / 6.6442000e-01 5.7064000e-01 2.3489000e-02 /
CHEB / -2.6436000e-01 1.5620000e-01 6.4608000e-02 /
CHEB / -2.6168000e-01 -9.0849000e-02 4.7490000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown10(10)     -91.93      99.72 32.17 39.92 46.93 52.67 61.88
      68.44 73.99 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
```

```
!Here are the path reactions and their high-P limit kinetics:
!     HCO+C4H9O-2=unknown10(10)     1.4157154e+13      -0.15000
2.9166667e+02
!     CO+nC4H10O=unknown10(10)      7.6600000e+05      2.07000
8.2200000e+04

HCO+C4H9O-2(+m)=CO+nC4H10O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #174 (unknown10)  deltaHrxn(T=298K) = -82.90142551012363
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2540000e+00 -1.4178000e+00 -3.7543000e-02 /
CHEB / 5.3620000e+00 9.8046000e-01 -4.2326000e-02 /
CHEB / 4.9428000e-01 5.5296000e-01 2.1449000e-02 /
CHEB / -3.3657000e-01 1.3852000e-01 5.5035000e-02 /
CHEB / -2.6396000e-01 -8.8788000e-02 3.7952000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -6.9  110.07      37.36 45.62 52.73 58.4  67.47
      74.43 82.92 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!     nSPC(102)         51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57
      23.05 null
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+nSPC(543)=unknown1(1)  7.9400000e+10      0.00000
6.7000000e+03
!     nC4H8O+nSPC(102)=unknown1(1)  7.9400000e+10      0.00000
6.7000000e+03

C3H7-1+nSPC(543)(+m)=nC4H8O+nSPC(102)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (unknown1)      deltaHrxn(T=298K) = -
5.439709477075475 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1564000e+00 -2.4060000e-01 -1.0972000e-01 /
CHEB / 2.2004000e+00 3.6345000e-01 1.5861000e-01 /
CHEB / -1.7686000e-01 -1.2571000e-01 -4.0394000e-02 /
CHEB / -6.4861000e-02 -2.7527000e-02 -2.5286000e-02 /
CHEB / -1.6141000e-02 3.3890000e-02 1.4188000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     unknown2(2)       -68.41      109.6 34.46 44.87 52.5  58.73 68.65
      75.89 82.36 null
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!     C3H7O2      -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67 54.73
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHO+C3H7O2=unknown2(2)     1.4157154e+13      -0.15000
2.9166667e+02
!     nSPC(543)+C3H7-1=unknown2(2)  1.4157154e+13      -0.15000
2.9166667e+02

nSPC(543)+C3H7-1(+m)=CH2CHO+C3H7O2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6 (unknown2)      deltaHrxn(T=298K) = -
10.748701621112033 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4880000e+00 -2.0158000e-07 -1.4032000e-07 /
CHEB / 6.9742000e-01 2.7285000e-07 1.8993000e-07 /
CHEB / 4.2791000e-01 -5.3343000e-08 -3.7131000e-08 /
CHEB / 7.7905000e-02 -3.2955000e-08 -2.2939000e-08 /
CHEB / -5.9547000e-03 1.3121000e-08 9.1329000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -113.93     121.68      42.27 54.44 63.04 69.81
      80.01 87.15 94.44 null
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     C3H7O2      -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67 54.73
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(801)+C3H7O2=unknown3(3)  1.4157154e+13      -0.15000
2.9166667e+02
!     nSPC(879)+C3H7-1=unknown3(3)  1.4157154e+13      -0.15000
2.9166667e+02

nSPC(879)+C3H7-1(+m)=nSPC(801)+C3H7O2(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #12 (unknown3)     deltaHrxn(T=298K) = -
2.7600551144343495 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3994000e-01 -3.9170000e-07 -2.7265000e-07 /
CHEB / 3.8507000e+00 5.8852000e-07 4.0965000e-07 /
CHEB / 8.0070000e-01 -2.2064000e-07 -1.5358000e-07 /
CHEB / 1.4057000e-01 4.6888000e-09 3.2637000e-09 /
CHEB / 8.7193000e-03 2.2987000e-08 1.6001000e-08 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       12.37 85.75 28.07 35.21 41.7  47.31 56.17 62.86
      74.32 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C4H8-1=unknown4(4)        1.3600000e+12      0.00000
1.0100000e+04
!     C3H6+C2H5=unknown4(4)         2.4827386e+10      0.24400
1.0487500e+04

CH3+C4H8-1(+m)=C3H6+C2H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #21 (unknown4)    deltaHrxn(T=298K) = -1.4594654173986754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0121000e+00 -8.5707000e-01 -1.5366000e-01 /
CHEB / 4.9302000e+00 9.8435000e-01 1.0766000e-01 /
CHEB / -1.1216000e-01 3.9556000e-02 1.0540000e-01 /
CHEB / -1.5926000e-01 -1.4630000e-01 -2.4340000e-02 /
CHEB / -4.6253000e-02 -6.3788000e-02 -4.6785000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -23.43      96.39 31.17 38.72 45.42 51.18 60.28
      67.03 76.51 null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!Here are the path reactions and their high-P limit kinetics:
!     C2H5+C3H6O-enol2=unknown5(5)  2.4827386e+10      0.24400
1.0487500e+04
!     C4H8-1+CH2OH=unknown5(5)      2.4827386e+10      0.24400
1.0487500e+04
```

```
C2H5+C3H6O-enol2(+m)=C4H8-1+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #29 (unknown5)     deltaHrxn(T=298K) = -
2.4594824867206193 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4874000e+00 -9.4198000e-01 -1.4333000e-01 /
CHEB / 4.7714000e+00 1.0143000e+00 7.3791000e-02 /
CHEB / -7.1503000e-02 1.1013000e-01 1.1284000e-01 /
CHEB / -1.6380000e-01 -1.2971000e-01 2.7073000e-03 /
CHEB / -7.6743000e-02 -7.8597000e-02 -3.9008000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -23.4 91.9  31.5  39.42 46.61 52.35 61.63 68.43
      79.02 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+CH3CHO=unknown6(6)     7.9400000e+10      0.00000
6.7000000e+03
!     nC4H8O+CH3=unknown6(6)        3.1600000e+10      0.00000
1.1510000e+04

nC4H8O+CH3(+m)=C3H7-1+CH3CHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #38 (unknown6)    deltaHrxn(T=298K) = 0.15064903989289036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9468000e+00 -6.6522000e-02 -4.1426000e-02 /
CHEB / 3.7966000e+00 9.8961000e-02 6.0944000e-02 /
CHEB / -2.3407000e-02 -3.2314000e-02 -1.8599000e-02 /
CHEB / 3.0250000e-02 -7.2282000e-03 -5.5200000e-03 /
CHEB / 2.0266000e-02 6.6560000e-03 3.9878000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -62.16      107.42      34.81 42.87 50.03 55.71
      64.96 71.66 80.14 null
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
```

```
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!Here are the path reactions and their high-P limit kinetics:
!     C2H5O-1+C3H6O-enol2=unknown7(7)     1.6297242e+02      2.92024
4.4628571e+04
!     C3H7O-N1+C2H4O=unknown7(7)    1.6297242e+02      2.92024
4.4628571e+04

C2H5O-1+C3H6O-enol2(+m)=C3H7O-N1+C2H4O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #47 (unknown7)    deltaHrxn(T=298K)
= -5.369199502263555 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5173000e+01 -6.9096000e-01 -1.9261000e-01 /
CHEB / 2.1038000e+01 8.1005000e-01 1.7100000e-01 /
CHEB / 1.2766000e+00 -2.0135000e-03 7.8699000e-02 /
CHEB / 2.5526000e-01 -1.0820000e-01 -3.3647000e-02 /
CHEB / 5.2841000e-02 -3.5812000e-02 -3.3579000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown8(8)       -70.99      95.36 31.98 40.04 47.27 53.5  63.36
      70.73 80.1  null
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9-1            20.65 78.53 23.01 28.55 33.6  37.94 44.89 50.17
      58.56
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H9O-1           -16.27      88.99 26.95 32.82 38.15 42.65 49.68
      54.93 63.28  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     nC3H7OH           -60.69      76.31 20.87 25.94 30.62 34.65 41.04
      45.85 53.48
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     CH2OH+C4H9-1=unknown8(8)      1.1500000e+13      0.00000
0.0000000e+00
!     C2H5O-1+C3H7-1=unknown8(8)    1.1500000e+13      0.00000
0.0000000e+00
!     C3H7O-N1+C2H5=unknown8(8)     1.1500000e+13      0.00000
0.0000000e+00
```

```
!     C4H9O-1+CH3=unknown8(8)       3.3700000e+13      0.00000
0.0000000e+00
!     nC3H7OH+C2H4=unknown8(8)      1.6297242e+02      2.92024
4.4628571e+04

CH2OH+C4H9-1(+m)=nC3H7OH+C2H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -63.94304896561385
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0456000e+00 -1.4714000e+00 -3.1786000e-02 /
CHEB / 2.9887000e+00 9.1752000e-01 -4.0943000e-02 /
CHEB / 3.5914000e-01 5.7776000e-01 7.0770000e-03 /
CHEB / -3.4155000e-01 2.1281000e-01 4.1231000e-02 /
CHEB / -3.1080000e-01 -3.2278000e-02 4.0153000e-02 /

C2H5O-1+C3H7-1(+m)=CH2OH+C4H9-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -2.609757135431554
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6582000e+00 -1.4014000e+00 -3.7462000e-02 /
CHEB / 3.9199000e+00 9.9867000e-01 -4.0334000e-02 /
CHEB / 3.5852000e-01 5.4337000e-01 2.5242000e-02 /
CHEB / -3.5547000e-01 1.1481000e-01 5.6229000e-02 /
CHEB / -2.4913000e-01 -1.0479000e-01 3.4488000e-02 /

C2H5O-1+C3H7-1(+m)=C3H7O-N1+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #54 (unknown8)     deltaHrxn(T=298K) = -
0.9599203294568248 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6192000e+00 -1.3942000e+00 -3.8308000e-02 /
CHEB / 4.0997000e+00 1.0061000e+00 -4.0351000e-02 /
CHEB / 3.3475000e-01 5.3791000e-01 2.7441000e-02 /
CHEB / -3.5805000e-01 1.0427000e-01 5.7689000e-02 /
CHEB / -2.4392000e-01 -1.1041000e-01 3.3447000e-02 /

C2H5O-1+C3H7-1(+m)=nC3H7OH+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -66.55280610104539
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3641000e+00 -1.4600000e+00 -3.2893000e-02 /
CHEB / 2.6755000e+00 9.3166000e-01 -4.1274000e-02 /
CHEB / 3.1164000e-01 5.7417000e-01 9.8014000e-03 /
CHEB / -3.3631000e-01 1.9792000e-01 4.4110000e-02 /
CHEB / -2.9773000e-01 -4.5347000e-02 4.0079000e-02 /

C3H7O-N1+C2H5(+m)=CH2OH+C4H9-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -1.6498368059747293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4150000e+00 -1.4039000e+00 -3.7157000e-02 /
CHEB / 4.1433000e+00 9.9605000e-01 -4.0314000e-02 /
CHEB / 3.5960000e-01 5.4523000e-01 2.4468000e-02 /
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CHEB / -3.6025000e-01 1.1850000e-01 5.5689000e-02 /
CHEB / -2.5283000e-01 -1.0276000e-01 3.4827000e-02 /

C3H7O-N1+C2H5(+m)=nC3H7OH+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -65.59288577158857
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1634000e+00 -1.4629000e+00 -3.2601000e-02 /
CHEB / 2.8512000e+00 9.2810000e-01 -4.1190000e-02 /
CHEB / 3.2279000e-01 5.7518000e-01 9.0829000e-03 /
CHEB / -3.3939000e-01 2.0176000e-01 4.3370000e-02 /
CHEB / -3.0219000e-01 -4.2078000e-02 4.0122000e-02 /

C4H9O-1+CH3(+m)=CH2OH+C4H9-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -2.169491137353887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0156000e+00 -1.4039000e+00 -3.7157000e-02 /
CHEB / 4.0544000e+00 9.9605000e-01 -4.0314000e-02 /
CHEB / 3.6718000e-01 5.4523000e-01 2.4468000e-02 /
CHEB / -3.4309000e-01 1.1850000e-01 5.5689000e-02 /
CHEB / -2.4213000e-01 -1.0276000e-01 3.4827000e-02 /

C4H9O-1+CH3(+m)=C2H5O-1+C3H7-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = 0.44026599807766686
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8414000e+00 -1.3942000e+00 -3.8308000e-02 /
CHEB / 4.3308000e+00 1.0061000e+00 -4.0351000e-02 /
CHEB / 3.3728000e-01 5.3791000e-01 2.7441000e-02 /
CHEB / -3.4381000e-01 1.0427000e-01 5.7689000e-02 /
CHEB / -2.3426000e-01 -1.1041000e-01 3.3447000e-02 /

C4H9O-1+CH3(+m)=C3H7O-N1+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -0.5196543313791615
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9711000e+00 -1.3967000e+00 -3.8002000e-02 /
CHEB / 4.2411000e+00 1.0035000e+00 -4.0340000e-02 /
CHEB / 3.4124000e-01 5.3985000e-01 2.6666000e-02 /
CHEB / -3.4544000e-01 1.0791000e-01 5.7183000e-02 /
CHEB / -2.3686000e-01 -1.0852000e-01 3.3817000e-02 /

C4H9O-1+CH3(+m)=nC3H7OH+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #54 (unknown8)    deltaHrxn(T=298K) = -66.11254010296773
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7641000e+00 -1.4629000e+00 -3.2601000e-02 /
CHEB / 2.7622000e+00 9.2810000e-01 -4.1190000e-02 /
CHEB / 3.3038000e-01 5.7518000e-01 9.0829000e-03 /
CHEB / -3.2223000e-01 2.0176000e-01 4.3370000e-02 /
CHEB / -2.9148000e-01 -4.2078000e-02 4.0122000e-02 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown9(9)       -72.43      92.67 31.71 39.98 47.34 53.64 63.55
      70.87 80.35 null
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9-2            18.01 78.98 21.99 27.3  32.36 36.82 44.06 49.58
      58.28
!     C3H7O-N2    -13.23      80.42 21.04 25.11 28.98 32.38 37.87 42.05
      48.76
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H9Oi1           -18.28      86.11 28.03 33.68 38.81 43.16 49.99
      55.12 63.33  !MRH
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     CH2OH+C4H9-2=unknown9(9)      4.7900000e+14      -0.75000
0.0000000e+00
!     C3H7O-N2+C2H5=unknown9(9)     1.1500000e+14      -0.35000
0.0000000e+00
!     C4H9O-3+CH3=unknown9(9)       6.6400000e+14      -0.57000
0.0000000e+00
!     C4H9Oi1+CH3=unknown9(9)       3.3700000e+13      0.00000
0.0000000e+00
!     CH3OH+C4H8-1=unknown9(9)      1.6297242e+02      2.92024
4.4628571e+04
!     C2H5OH+C3H6=unknown9(9)       1.6297242e+02      2.92024
4.4628571e+04

CH2OH+C4H9-2(+m)=CH3OH+C4H8-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -60.753579337011914
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9365000e+00 -1.3919000e+00 -4.4067000e-02 /
CHEB / 2.6520000e+00 1.0107000e+00 -4.6143000e-02 /
CHEB / 2.6420000e-01 5.4199000e-01 3.2652000e-02 /
CHEB / -3.4154000e-01 1.0401000e-01 6.9217000e-02 /
CHEB / -2.5544000e-01 -1.1666000e-01 4.1111000e-02 /
```

```
CH2OH+C4H9-2(+m)=C2H5OH+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -64.1631602924973
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5468000e+00 -1.3983000e+00 -4.3558000e-02 /
CHEB / 2.3455000e+00 1.0043000e+00 -4.6383000e-02 /
CHEB / 2.0183000e-01 5.4744000e-01 3.0877000e-02 /
CHEB / -3.5359000e-01 1.1419000e-01 6.8340000e-02 /
CHEB / -2.6565000e-01 -1.1147000e-01 4.2380000e-02 /

C3H7O-N2+C2H5(+m)=CH2OH+C4H9-2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -2.029806637624766
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6586000e+00 -1.3381000e+00 -4.9800000e-02 /
CHEB / 3.2027000e+00 1.0584000e+00 -4.3853000e-02 /
CHEB / 1.4183000e-01 4.8986000e-01 4.9201000e-02 /
CHEB / -3.8443000e-01 2.4871000e-02 7.4238000e-02 /
CHEB / -2.2896000e-01 -1.4608000e-01 2.7183000e-02 /

C3H7O-N2+C2H5(+m)=CH3OH+C4H8-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -62.78338597463669
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5291000e+00 -1.3815000e+00 -4.5548000e-02 /
CHEB / 2.7157000e+00 1.0204000e+00 -4.6080000e-02 /
CHEB / 2.7350000e-01 5.3278000e-01 3.6249000e-02 /
CHEB / -3.1362000e-01 8.8712000e-02 7.1170000e-02 /
CHEB / -2.3693000e-01 -1.2339000e-01 3.9022000e-02 /

C3H7O-N2+C2H5(+m)=C2H5OH+C3H6(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -66.19296693012207
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1180000e+00 -1.3877000e+00 -4.5085000e-02 /
CHEB / 2.4309000e+00 1.0144000e+00 -4.6384000e-02 /
CHEB / 2.0903000e-01 5.3842000e-01 3.4553000e-02 /
CHEB / -3.2726000e-01 9.8582000e-02 7.0539000e-02 /
CHEB / -2.4685000e-01 -1.1879000e-01 4.0457000e-02 /

C4H9O-3+CH3(+m)=CH2OH+C4H9-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -2.5790915622304844
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9394000e+00 -1.3381000e+00 -4.9800000e-02 /
CHEB / 3.0240000e+00 1.0584000e+00 -4.3853000e-02 /
CHEB / 1.2658000e-01 4.8986000e-01 4.9201000e-02 /
CHEB / -3.6114000e-01 2.4871000e-02 7.4238000e-02 /
CHEB / -2.1455000e-01 -1.4608000e-01 2.7183000e-02 /
```

```
C4H9O-3+CH3(+m)=C3H7O-N2+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -0.5492849246057183
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3551000e+00 -1.3287000e+00 -5.1011000e-02 /
CHEB / 3.5124000e+00 1.0656000e+00 -4.3280000e-02 /
CHEB / 1.5978000e-01 4.7947000e-01 5.2307000e-02 /
CHEB / -3.4120000e-01 1.2266000e-02 7.4510000e-02 /
CHEB / -2.0094000e-01 -1.4874000e-01 2.4233000e-02 /

C4H9O-3+CH3(+m)=CH3OH+C4H8-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -63.3326708992424
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8099000e+00 -1.3815000e+00 -4.5548000e-02 /
CHEB / 2.5370000e+00 1.0204000e+00 -4.6080000e-02 /
CHEB / 2.5825000e-01 5.3278000e-01 3.6249000e-02 /
CHEB / -2.9033000e-01 8.8712000e-02 7.1170000e-02 /
CHEB / -2.2251000e-01 -1.2339000e-01 3.9022000e-02 /

C4H9O-3+CH3(+m)=C2H5OH+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -66.74225185472778
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3989000e+00 -1.3877000e+00 -4.5085000e-02 /
CHEB / 2.2522000e+00 1.0144000e+00 -4.6384000e-02 /
CHEB / 1.9378000e-01 5.3842000e-01 3.4553000e-02 /
CHEB / -3.0397000e-01 9.8582000e-02 7.0539000e-02 /
CHEB / -2.3243000e-01 -1.1879000e-01 4.0457000e-02 /

C4H9Oi1+CH3(+m)=CH2OH+C4H9-2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -2.799125995265868
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2602000e+00 -1.3381000e+00 -4.9800000e-02 /
CHEB / 3.2860000e+00 1.0584000e+00 -4.3853000e-02 /
CHEB / 1.9951000e-01 4.8986000e-01 4.9201000e-02 /
CHEB / -3.3581000e-01 2.4871000e-02 7.4238000e-02 /
CHEB / -2.0165000e-01 -1.4608000e-01 2.7183000e-02 /

C4H9Oi1+CH3(+m)=C3H7O-N2+C2H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -0.7693193576411055
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6758000e+00 -1.3287000e+00 -5.1011000e-02 /
CHEB / 3.7744000e+00 1.0656000e+00 -4.3280000e-02 /
CHEB / 2.3271000e-01 4.7947000e-01 5.2307000e-02 /
CHEB / -3.1587000e-01 1.2266000e-02 7.4510000e-02 /
CHEB / -1.8804000e-01 -1.4874000e-01 2.4233000e-02 /
```

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C4H9Oi1+CH3(+m)=C4H9O-3+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -0.22003443303538717
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9931000e+00 -1.3287000e+00 -5.1011000e-02 /
CHEB / 4.0924000e+00 1.0656000e+00 -4.3280000e-02 /
CHEB / 3.1628000e-01 4.7947000e-01 5.2307000e-02 /
CHEB / -2.8659000e-01 1.2266000e-02 7.4510000e-02 /
CHEB / -1.7652000e-01 -1.4874000e-01 2.4233000e-02 /

C4H9Oi1+CH3(+m)=CH3OH+C4H8-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -63.55270533227778
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1307000e+00 -1.3815000e+00 -4.5548000e-02 /
CHEB / 2.7990000e+00 1.0204000e+00 -4.6080000e-02 /
CHEB / 3.3118000e-01 5.3278000e-01 3.6249000e-02 /
CHEB / -2.6500000e-01 8.8712000e-02 7.1170000e-02 /
CHEB / -2.0962000e-01 -1.2339000e-01 3.9022000e-02 /

C4H9Oi1+CH3(+m)=C2H5OH+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -66.96228628776316
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7196000e+00 -1.3877000e+00 -4.5085000e-02 /
CHEB / 2.5142000e+00 1.0144000e+00 -4.6384000e-02 /
CHEB / 2.6671000e-01 5.3842000e-01 3.4553000e-02 /
CHEB / -2.7864000e-01 9.8582000e-02 7.0539000e-02 /
CHEB / -2.1954000e-01 -1.1879000e-01 4.0457000e-02 /

CH3OH+C4H8-1(+m)=C2H5OH+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #55 (unknown9)    deltaHrxn(T=298K) = -3.409580955485384
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3690000e+01 -1.4484000e+00 -3.7458000e-02 /
CHEB / 2.0998000e+01 9.5071000e-01 -4.5875000e-02 /
CHEB / 8.1347000e-01 5.8184000e-01 1.4744000e-02 /
CHEB / -2.8828000e-01 1.9084000e-01 5.4895000e-02 /
CHEB / -2.9679000e-01 -6.3750000e-02 4.7011000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown10(10)     -75.36      93.36 32.48 40.72 48.22 54.24 64.01
      71.23 82.61 null
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
```

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!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C2H5O-2+C3H7-1=unknown10(10)  4.7900000e+14      -0.75000
0.0000000e+00
!     C4H9O-4+CH3=unknown10(10)     6.8000000e+14      -0.68000
0.0000000e+00
!     C2H5OH+C3H6=unknown10(10)     1.6297242e+02      2.92024
4.4628571e+04

C2H5O-2+C3H7-1(+m)=C2H5OH+C3H6(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #56 (unknown10)   deltaHrxn(T=298K) = -62.283402169932636
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3035000e+00 -1.4235000e+00 -4.6150000e-02 /
CHEB / 2.4498000e+00 9.7215000e-01 -5.2086000e-02 /
CHEB / 3.4470000e-01 5.5436000e-01 2.5251000e-02 /
CHEB / -2.6292000e-01 1.4812000e-01 6.6908000e-02 /
CHEB / -2.3620000e-01 -8.0134000e-02 4.8106000e-02 /

C4H9O-4+CH3(+m)=C2H5O-2+C3H7-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #56 (unknown10)   deltaHrxn(T=298K) = 0.17038616460624212
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4404000e+00 -1.3779000e+00 -5.0800000e-02 /
CHEB / 3.2961000e+00 1.0176000e+00 -5.0037000e-02 /
CHEB / 2.3557000e-01 5.1940000e-01 4.0429000e-02 /
CHEB / -3.2043000e-01 8.2828000e-02 7.4725000e-02 /
CHEB / -2.2023000e-01 -1.1457000e-01 3.8796000e-02 /

C4H9O-4+CH3(+m)=C2H5OH+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #56 (unknown10)   deltaHrxn(T=298K) = -62.113016005326394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6941000e+00 -1.4260000e+00 -4.5779000e-02 /
CHEB / 2.4848000e+00 9.6955000e-01 -5.2083000e-02 /
CHEB / 3.7252000e-01 5.5607000e-01 2.4329000e-02 /
CHEB / -2.4033000e-01 1.5165000e-01 6.6234000e-02 /
CHEB / -2.2480000e-01 -7.8040000e-02 4.8431000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -65.33      91.78 32.27 40.81 48.25 54.25 64.35
      71.65 83.1  null
```

```
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-1+CH3OH=unknown1(1)      2.4800000e+01      2.93000
4.3900000e+04
!     C4H8-2+CH3OH=unknown1(1)      1.1691492e+02      2.87714
4.8857143e+04

C4H8-1+CH3OH(+m)=C4H8-2+CH3OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (unknown1)     deltaHrxn(T=298K) = -2.719803185470056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5194000e+01 -1.5439000e+00 -3.2928000e-02 /
CHEB / 2.1801000e+01 8.1968000e-01 -4.8891000e-02 /
CHEB / 9.6987000e-01 5.8231000e-01 -9.2116000e-03 /
CHEB / -2.4609000e-01 2.9671000e-01 2.8493000e-02 /
CHEB / -3.4546000e-01 6.0583000e-02 4.4835000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -108.23     103.32      34.81 43.49 51.06 57.51
      67.66 75.04 82.54 null
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-3+CH2OH=unknown2(2)     4.7900000e+14      -0.75000
0.0000000e+00
!     C2H5OH+C3H6O-enol2=unknown2(2)      1.6297242e+02      2.92024
4.4628571e+04

C4H9O-3+CH2OH(+m)=C2H5OH+C3H6O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (unknown2)      deltaHrxn(T=298K) = -
62.82330395060849 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4064000e+00 -1.4283000e+00 -3.5208000e-02 /
CHEB / 3.6741000e+00 9.7720000e-01 -4.0362000e-02 /
CHEB / 3.8413000e-01 5.7900000e-01 2.0676000e-02 /
CHEB / -3.4682000e-01 1.6676000e-01 5.6928000e-02 /
CHEB / -2.9291000e-01 -8.8672000e-02 4.1894000e-02 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -111.16     104.01      35.58 44.23 51.94 58.11
      68.12 75.4  84.8  null
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-4+CH2OH=unknown3(3)     4.7900000e+14      -0.75000
0.0000000e+00
!     C2H5OH+C3H6O-enol2=unknown3(3)      1.6297242e+02      2.92024
4.4628571e+04

C4H9O-4+CH2OH(+m)=C2H5OH+C3H6O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (unknown3)      deltaHrxn(T=298K) = -
58.19406810120711 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5664000e+00 -1.4191000e+00 -3.9167000e-02 /
CHEB / 4.0560000e+00 9.8723000e-01 -4.3298000e-02 /
CHEB / 4.8889000e-01 5.7312000e-01 2.6689000e-02 /
CHEB / -3.2471000e-01 1.5264000e-01 6.5797000e-02 /
CHEB / -2.7246000e-01 -9.8151000e-02 4.4922000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       37.4  91.77 28.77 37.7  45.67 51.42 60.65 66.99
      79.95 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+aC3H5=unknown4(4) 6.9200000e+10      0.00000
4.3720000e+04
!     C4H6-13+CH2CHO=unknown4(4)    6.9200000e+10      0.00000
4.3720000e+04

C4H6-13+CH2CHO(+m)=C3H4O+aC3H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (unknown4)     deltaHrxn(T=298K) = -5.859548119682479
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9913000e+00 -1.6934000e-01 -9.8467000e-02 /
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CHEB / 1.6506000e+01 2.2327000e-01 1.2553000e-01 /
CHEB / 3.6248000e-01 -4.0198000e-02 -1.5719000e-02 /
CHEB / 9.1865000e-03 -1.9438000e-02 -1.4328000e-02 /
CHEB / -3.9808000e-02 2.2759000e-03 2.7771000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -18.96      98.93 32.41 40.96 48.23 53.89 62.92
      69.33 78.44 null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+C3H5O-enol2=unknown5(5) 4.7900000e+14      -0.75000
0.0000000e+00
!     C2H4O+C4H6-13=unknown5(5)     1.6297242e+02      2.92024
4.4628571e+04

aC3H5+C3H5O-enol2(+m)=C2H4O+C4H6-13(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #26 (unknown5)     deltaHrxn(T=298K) = -
40.82584518005103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7821000e+00 -1.4409000e+00 -4.5669000e-02 /
CHEB / 5.9785000e+00 9.5069000e-01 -5.3962000e-02 /
CHEB / 7.7419000e-01 5.6040000e-01 1.9508000e-02 /
CHEB / -1.3366000e-01 1.7357000e-01 6.1661000e-02 /
CHEB / -1.7709000e-01 -5.6855000e-02 4.8804000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -16.79      96.22 33.68 43.18 50.92 56.65 65.47
      71.92 80.86 null
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!Here are the path reactions and their high-P limit kinetics:
!     C4H7-24+CH2CHO=unknown6(6)    1.4157154e+13      -0.15000
2.9166667e+02
!     C4H6-13+C2H4O=unknown6(6)     1.1691492e+02      2.87714
4.8857143e+04
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```
C4H7-24+CH2CHO(+m)=C4H6-13+C2H4O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #77 (unknown6)     deltaHrxn(T=298K) = -
39.696058228343276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5236000e+00 -1.2450000e+00 -7.2881000e-02 /
CHEB / 6.5115000e+00 1.0776000e+00 -2.7859000e-02 /
CHEB / 5.7389000e-01 3.7432000e-01 8.0996000e-02 /
CHEB / -5.4033000e-02 -3.4973000e-02 6.2525000e-02 /
CHEB / -6.1090000e-02 -1.1820000e-01 9.5956000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -11.6 88.36 29.54 39.06 47.58 53.82 63.81 70.73
      84.61 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C3H6=unknown7(7)  6.9200000e+10      0.00000
4.3720000e+04
!     C4H6-13+CH3CHO=unknown7(7)    6.9200000e+10      0.00000
4.3720000e+04

C3H4O+C3H6(+m)=C4H6-13+CH3CHO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #130 (unknown7)   deltaHrxn(T=298K) = -2.3295946307222692
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4468000e+00 -1.2619000e+00 -5.8349000e-02 /
CHEB / 1.7164000e+01 1.0999000e+00 -3.1146000e-02 /
CHEB / -3.4419000e-02 4.0072000e-01 7.3107000e-02 /
CHEB / -2.7642000e-01 -4.7983000e-02 6.4764000e-02 /
CHEB / -1.1786000e-01 -1.4319000e-01 7.7589000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown8(8)       41.14 84.67 27.31 36.43 44.58 51.28 61.65 69.1
      81.49 null
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
```

```
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C4H7-24+C2H4=unknown8(8)      6.9200000e+10      0.00000
4.3720000e+04
!     aC3H5+C3H6=unknown8(8)  6.9200000e+10      0.00000
4.3720000e+04

C4H7-24+C2H4(+m)=aC3H5+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #171 (unknown8)   deltaHrxn(T=298K) = -0.050005963314698754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0775000e+01 -9.8624000e-01 -1.5185000e-01 /
CHEB / 1.7687000e+01 9.8755000e-01 6.2260000e-02 /
CHEB / 1.1092000e-01 1.8273000e-01 1.1724000e-01 /
CHEB / -2.3976000e-01 -9.6895000e-02 2.7712000e-02 /
CHEB / -1.4667000e-01 -9.0305000e-02 -3.1168000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown9(9)       37.04 93.48 30.76 38.67 45.79 51.66 61.02 67.95
      79.66 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C4H8-1=unknown9(9) 1.4902950e+02      3.00740
1.0170800e+04
!     C4H6-13+C2H5=unknown9(9)      7.2517543e+09      0.48800
1.0375000e+04

C2H3+C4H8-1(+m)=C4H6-13+C2H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (unknown9)   deltaHrxn(T=298K) = -15.69828967598723
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5138000e+00 -8.8268000e-01 -1.8036000e-01 /
CHEB / 5.4303000e+00 9.3691000e-01 1.1412000e-01 /
CHEB / 2.9059000e-01 1.1807000e-01 1.1507000e-01 /
CHEB / -6.7976000e-02 -1.1442000e-01 -8.0080000e-05 /
CHEB / -7.1001000e-02 -8.0486000e-02 -4.2024000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
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!     unknown10(10)     0.97  93.32 30.91 40.62 49.25 55.89 66.41 73.77
      86.19 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!Here are the path reactions and their high-P limit kinetics:
!     C3H6+C3H5O-enol2=unknown10(10)      6.9200000e+10      0.00000
4.3720000e+04
!     C4H7-24+C2H4O=unknown10(10)   6.9200000e+10      0.00000
4.3720000e+04

C4H7-24+C2H4O(+m)=C3H6+C3H5O-enol2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #240 (unknown10)   deltaHrxn(T=298K) = -
0.7997991543552956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0868000e+01 -7.2961000e-01 -1.9564000e-01 /
CHEB / 1.7742000e+01 8.3056000e-01 1.6155000e-01 /
CHEB / 2.5718000e-01 2.4285000e-02 8.9696000e-02 /
CHEB / -1.3213000e-01 -1.0412000e-01 -2.5384000e-02 /
CHEB / -1.0155000e-01 -4.4017000e-02 -3.5611000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown11(11)     6.17  90.83 30.74 40.64 49.49 56.32 67.11 74.67
      86.19 null
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     CH2CHO      4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19 27.35
!Here are the path reactions and their high-P limit kinetics:
!     C4H7OJ(12)+C2H4=unknown11(11) 6.9200000e+10      0.00000
4.3720000e+04
!     C4H8-1+CH2CHO=unknown11(11)   6.9200000e+10      0.00000
4.3720000e+04

C4H7OJ(12)+C2H4(+m)=C4H8-1+CH2CHO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #287 (unknown11)   deltaHrxn(T=298K) = -
0.5799669394682665 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2098000e+01 -1.5810000e-04 -1.1004000e-04 /
CHEB / 1.8071000e+01 1.7352000e-04 1.2076000e-04 /
CHEB / 8.3773000e-01 4.0037000e-06 2.7902000e-06 /
CHEB / 1.2747000e-01 -1.8035000e-05 -1.2552000e-05 /
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CHEB / -1.5607000e-02 -3.6512000e-06 -2.5421000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown12(12)     -10.44      97.79 35.07 44.72 52.62 58.93 68.45
      75.56 84.13 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C3H7-1=unknown12(12)    2.3501400e+11      0.30815
4.9629937e+03
!     C3H5O-enol2+C3H6=unknown12(12)      1.1691492e+02      2.87714
4.8857143e+04

C3H4O+C3H7-1(+m)=C3H5O-enol2+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #342 (unknown12)   deltaHrxn(T=298K) = -
6.149312741335112 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8124000e+00 -2.2450000e-05 -1.9087000e-05 /
CHEB / 1.5512000e+01 1.9649000e-05 1.6686000e-05 /
CHEB / 4.9333000e-02 1.4362000e-05 1.2233000e-05 /
CHEB / -1.4245000e-01 -1.1390000e-05 -9.5973000e-06 /
CHEB / -1.8111000e-01 -6.1451000e-06 -5.1024000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown13(13)     2.85  99.16 34.24 43.15 50.88 57.0  66.76 73.78
      83.76 null
!     nC4H8O            -49.43      82.15 24.92 30.36 35.17 39.32 46.39
      51.51 58.1  null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!Here are the path reactions and their high-P limit kinetics:
!     nC4H8O+C2H3=unknown13(13)     3.2847733e+07      1.50370
7.3354000e+03
!     C3H7-1+C3H4O=unknown13(13)    7.9400000e+10      0.00000
6.7000000e+03

nC4H8O+C2H3(+m)=C3H7-1+C3H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #421 (unknown13)  deltaHrxn(T=298K) = -11.758580587973393
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6657000e+00 -6.9358000e-02 -4.8216000e-02 /
CHEB / 2.4919000e+00 1.0221000e-01 7.0369000e-02 /
CHEB / -2.5271000e-01 -3.0007000e-02 -1.9287000e-02 /
CHEB / -1.7686000e-01 -1.2413000e-02 -9.6972000e-03 /
CHEB / -8.3832000e-02 8.6126000e-03 5.6745000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown14(14)     -46.24      108.43      38.17 48.23 56.34 62.8
      72.56 79.73 86.32 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C3H7O-N1=unknown14(14)  2.3501400e+11      0.30815
4.9629937e+03
!     C3H5O-enol2+C3H6O-enol2=unknown14(14)     1.1691492e+02
2.87714      4.8857143e+04

C3H4O+C3H7O-N1(+m)=C3H5O-enol2+C3H6O-enol2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #538 (unknown14)  deltaHrxn(T=298K)
= -5.139655701059034 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.2900000e+00 -1.1214000e-03 -9.5030000e-04 /
CHEB / 1.6269000e+01 1.4910000e-03 1.2636000e-03 /
CHEB / 3.4153000e-01 -1.7990000e-04 -1.5275000e-04 /
CHEB / 9.5973000e-02 -3.3426000e-04 -2.8294000e-04 /
CHEB / 8.2269000e-03 1.0323000e-04 8.7372000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-2+C2H4=unknown15(15)     6.9200000e+10      0.00000
4.3720000e+04
!     C3H6+C3H6=unknown15(15)       6.9200000e+10      0.00000
4.3720000e+04
```

```
C4H8-2+C2H4(+m)=C3H6+C3H6(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #632 (unknown15)  deltaHrxn(T=298K) = -0.22986638790468383
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0709000e+01 -1.3111000e+00 -4.6692000e-02 /
CHEB / 1.8026000e+01 1.0780000e+00 -3.5248000e-02 /
CHEB / 3.3361000e-02 4.6014000e-01 5.3211000e-02 /
CHEB / -3.5087000e-01 -5.6986000e-03 6.4013000e-02 /
CHEB / -1.5900000e-01 -1.4853000e-01 1.2911000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown16(16)     -47.76      100.41      34.4  43.44 51.43 57.99
      68.4  75.96 85.69 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C4H9O-3=unknown16(16)    1.4157154e+13      -0.15000
2.9166667e+02
!     C4H6-13+C2H5OH=unknown16(16)  1.6297242e+02      2.92024
4.4628571e+04
!     C2H4O+C4H8-1=unknown16(16)    1.6297242e+02      2.92024
4.4628571e+04

C2H3+C4H9O-3(+m)=C4H6-13+C2H5OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #653 (unknown16)  deltaHrxn(T=298K) = -80.98107611331633
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4435000e+00 -1.3055000e+00 -6.6854000e-02 /
CHEB / 2.3456000e+00 1.0596000e+00 -4.0174000e-02 /
CHEB / 3.1210000e-01 4.5358000e-01 7.0088000e-02 /
CHEB / -1.4636000e-01 1.2856000e-02 7.9227000e-02 /
CHEB / -1.4243000e-01 -1.3261000e-01 1.8950000e-02 /

C2H3+C4H9O-3(+m)=C2H4O+C4H8-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #653 (unknown16)  deltaHrxn(T=298K) = -80.93137424635334
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1871000e+00 -1.3055000e+00 -6.6854000e-02 /
CHEB / 2.2810000e+00 1.0596000e+00 -4.0174000e-02 /
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CHEB / 2.9512000e-01 4.5358000e-01 7.0088000e-02 /
CHEB / -1.5231000e-01 1.2856000e-02 7.9227000e-02 /
CHEB / -1.4477000e-01 -1.3261000e-01 1.8950000e-02 /

C4H6-13+C2H5OH(+m)=C2H4O+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #653 (unknown16)  deltaHrxn(T=298K) = 0.049701866962998054
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4843000e+01 -1.4629000e+00 -3.1000000e-02 /
CHEB / 2.2379000e+01 9.3680000e-01 -3.9125000e-02 /
CHEB / 1.0236000e+00 5.9728000e-01 9.6495000e-03 /
CHEB / -2.1808000e-01 2.2064000e-01 4.4063000e-02 /
CHEB / -2.7611000e-01 -4.7426000e-02 4.0582000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown17(17)     -47.97      98.38 36.44 46.4  54.9  61.35 71.41
      78.91 90.37 null
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H4O       -29.12      62.18 15.02 18.07 20.54 22.51 25.45 27.61
      31.14
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-1+C2H4O=unknown17(17)    1.1691492e+02      2.87714
4.8857143e+04
!     C4H8-2+C2H4O=unknown17(17)    1.1691492e+02      2.87714
4.8857143e+04

C4H8-1+C2H4O(+m)=C4H8-2+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #760 (unknown17)  deltaHrxn(T=298K) = -2.719803185470056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7179000e+01 -1.4338000e+00 -3.9707000e-02 /
CHEB / 2.2951000e+01 9.5910000e-01 -4.6567000e-02 /
CHEB / 9.4189000e-01 5.5567000e-01 1.7874000e-02 /
CHEB / -1.6524000e-01 1.6034000e-01 5.3828000e-02 /
CHEB / -2.0706000e-01 -6.6371000e-02 4.1041000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown18(18)     -47.76      100.41      34.4  43.44 51.43 57.99
      68.4  75.96 85.69 null
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
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!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C4H9O-2=unknown18(18)    1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7-24+C2H5O-1=unknown18(18) 4.7900000e+14      -0.75000
0.0000000e+00

C2H3+C4H9O-2(+m)=C4H7-24+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #837 (unknown18)   deltaHrxn(T=298K) = -
23.507449692272296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0512000e+01 -1.3229000e+00 -5.9934000e-02 /
CHEB / 1.6085000e+00 1.0521000e+00 -4.2764000e-02 /
CHEB / 1.2931000e-01 4.6390000e-01 6.0302000e-02 /
CHEB / -2.7274000e-01 2.3905000e-02 7.4137000e-02 /
CHEB / -1.9958000e-01 -1.2635000e-01 2.1225000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown19(19)     -49.11      100.62      35.22 44.45 52.49 58.89
      69.14 76.58 87.35 null
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     C2H3        72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05 21.77
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-4+C2H3=unknown19(19)    1.4157154e+13      -0.15000
2.9166667e+02
!     C3H7-1+C3H5O-enol2=unknown19(19)    4.7900000e+14      -0.75000
0.0000000e+00
!     C2H5OH+C4H6-13=unknown19(19)  1.6297242e+02      2.92024
4.4628571e+04

C4H9O-4+C2H3(+m)=C3H7-1+C3H5O-enol2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #960 (unknown19)   deltaHrxn(T=298K) = -
25.237309014235638 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0316000e+01 -1.3490000e+00 -5.8349000e-02 /
CHEB / 1.6112000e+00 1.0330000e+00 -4.6552000e-02 /
CHEB / 7.2301000e-02 4.9171000e-01 5.3923000e-02 /
CHEB / -3.0561000e-01 5.7788000e-02 7.6874000e-02 /
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CHEB / -2.2335000e-01 -1.1731000e-01 2.9940000e-02 /

C4H9O-4+C2H3(+m)=C2H5OH+C4H6-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #960 (unknown19)  deltaHrxn(T=298K) = -76.35184026391497
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9051000e+00 -1.3620000e+00 -5.6498000e-02 /
CHEB / 2.6797000e+00 1.0232000e+00 -4.7320000e-02 /
CHEB / 3.4604000e-01 5.0566000e-01 4.9609000e-02 /
CHEB / -1.9484000e-01 7.5821000e-02 7.6084000e-02 /
CHEB / -1.8320000e-01 -1.1183000e-01 3.3403000e-02 /

C3H7-1+C3H5O-enol2(+m)=C2H5OH+C4H6-13(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #960 (unknown19)   deltaHrxn(T=298K) = -
51.11453124967932 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7650000e+00 -1.4678000e+00 -3.6379000e-02 /
CHEB / 4.5264000e+00 9.2627000e-01 -4.6754000e-02 /
CHEB / 6.0253000e-01 5.8793000e-01 8.6001000e-03 /
CHEB / -3.2766000e-01 2.1861000e-01 4.8174000e-02 /
CHEB / -3.1941000e-01 -3.8065000e-02 4.6639000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown20(20)     -25.94      109.91      38.86 48.51 56.79 63.74
      74.78 83.24 92.97 null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C3H7O2      -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67 54.73
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+C3H7O2=unknown20(20)    1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5O2+C3H7-1=unknown20(20)  1.4157154e+13      -0.15000
2.9166667e+02

aC3H5O2+C3H7-1(+m)=aC3H5+C3H7O2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1093 (unknown20) deltaHrxn(T=298K) = -15.6382998491827
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3752000e+00 -3.7747000e-06 -2.6275000e-06 /
CHEB / 1.4575000e+00 5.6799000e-06 3.9537000e-06 /
CHEB / 3.9556000e-01 -2.0862000e-06 -1.4522000e-06 /
CHEB / 6.3890000e-02 -8.1430000e-08 -5.6678000e-08 /
CHEB / -1.1985000e-02 3.1991000e-07 2.2268000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
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!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -113.51     127.67      43.56 56.01 65.42 72.69
      84.48 92.9  101.31      null
!     nSPC(301)         -53.93      102.11      32.84 39.97 46.09 50.94
      58.78 64.89 72.26 null
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     nSPC(543)         -18.09      77.55 19.79 23.22 26.1  28.39 31.7
      33.97 37.29
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(301)+CH2CHO=unknown1(1)  1.4157154e+13      -0.15000
2.9166667e+02
!     C4H9O-2+nSPC(543)=unknown1(1) 6.0300000e+12      0.00000
0.0000000e+00

C4H9O-2+nSPC(543)(+m)=nSPC(301)+CH2CHO(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (unknown1)     deltaHrxn(T=298K)
= -11.388627055318523 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3024000e+00 -6.2692000e-01 -1.9274000e-01 /
CHEB / 2.6973000e+00 7.2968000e-01 1.8242000e-01 /
CHEB / 4.9540000e-01 5.1247000e-03 5.9862000e-02 /
CHEB / -1.8790000e-02 -9.9466000e-02 -3.0000000e-02 /
CHEB / -6.4209000e-02 -3.1611000e-02 -2.7421000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown2(2)       -159.03     139.75      51.37 65.58 75.96 83.77
      95.84 104.16      113.39      null
!     nSPC(301)         -53.93      102.11      32.84 39.97 46.09 50.94
      58.78 64.89 72.26 null
!     nSPC(801)         -34.67      73.73 21.04 25.44 28.98 31.67 35.2
      37.28 39.6
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     nSPC(879)         -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55
      47.83 null
!Here are the path reactions and their high-P limit kinetics:
!     nSPC(301)+nSPC(801)=unknown2(2)     1.4157154e+13      -0.15000
2.9166667e+02
!     C4H9O-2+nSPC(879)=unknown2(2) 6.0300000e+12      0.00000
0.0000000e+00

C4H9O-2+nSPC(879)(+m)=nSPC(301)+nSPC(801)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4 (unknown2)     deltaHrxn(T=298K)
= -3.3999805486408334 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 4.8311000e+00 -5.5228000e-01 -1.7574000e-01 /
CHEB / 5.2668000e+00 6.9690000e-01 1.8717000e-01 /
CHEB / 7.4802000e-01 -6.7659000e-02 3.5240000e-02 /
CHEB / 4.5975000e-02 -9.1953000e-02 -4.1733000e-02 /
CHEB / -1.6671000e-02 -7.0819000e-03 -1.7595000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(3)       -24.53      105.0 36.49 46.3  54.64 61.28 72.29
      80.24 90.77 null
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-1+C2H5O-1=unknown3(3)    2.4800000e+01      2.93000
4.3900000e+04
!     C4H8-2+C2H5O-1=unknown3(3)    1.1691492e+02      2.87714
4.8857143e+04

C4H8-1+C2H5O-1(+m)=C4H8-2+C2H5O-1(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #11 (unknown3)     deltaHrxn(T=298K) = -
2.7198031854700546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7589000e+01 -7.7390000e-01 -2.0081000e-01 /
CHEB / 2.2188000e+01 8.2905000e-01 1.5800000e-01 /
CHEB / 1.0146000e+00 1.0544000e-01 9.5590000e-02 /
CHEB / 8.0124000e-02 -1.1510000e-01 -1.2242000e-02 /
CHEB / -2.5227000e-03 -7.6306000e-02 -4.1777000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown4(4)       -75.92      104.78      37.48 46.99 55.52 62.85
      74.43 83.07 94.35 null
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+C3H7O-N1=unknown4(4)   1.1500000e+13      0.00000
0.0000000e+00
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```
!     nC4H10O+C2H4=unknown4(4)      1.6297242e+02      2.92024
4.4628571e+04

C3H7-1+C3H7O-N1(+m)=nC4H10O+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (unknown4)     deltaHrxn(T=298K) = -
66.7729848964456 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1302000e+00 -1.4735000e+00 -2.8419000e-02 /
CHEB / 3.9572000e+00 9.2327000e-01 -3.7564000e-02 /
CHEB / 4.9312000e-01 5.9982000e-01 4.5912000e-03 /
CHEB / -3.8983000e-01 2.3402000e-01 3.6966000e-02 /
CHEB / -3.6761000e-01 -3.4780000e-02 3.8538000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown5(5)       -69.66      103.57      36.76 46.98 55.6  62.94
      74.8  83.48 92.92 null
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!Here are the path reactions and their high-P limit kinetics:
!     nC4H10O+C2H4=unknown5(5)      4.7300000e+01      3.00000
4.7000000e+04
!     C4H8-1+C2H5OH=unknown5(5)     1.1691492e+02      2.87714
4.8857143e+04

nC4H10O+C2H4(+m)=C4H8-1+C2H5OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #14 (unknown5)    deltaHrxn(T=298K) = -1.8196557268888611
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6251000e+01 -1.5435000e+00 -2.9232000e-02 /
CHEB / 2.3294000e+01 8.2526000e-01 -4.4771000e-02 /
CHEB / 1.0586000e+00 5.9635000e-01 -1.1815000e-02 /
CHEB / -3.1940000e-01 3.1058000e-01 2.1941000e-02 /
CHEB / -4.4057000e-01 6.0384000e-02 4.0524000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown6(6)       -80.29      102.78      37.98 47.67 56.47 63.59
      75.08 83.57 96.86 null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
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!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-4+C2H5=unknown6(6)      4.7900000e+14      -0.75000
0.0000000e+00
!     C2H5OH+C4H8-1=unknown6(6)     1.6297242e+02      2.92024
4.4628571e+04

C4H9O-4+C2H5(+m)=C2H5OH+C4H8-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #15 (unknown6)    deltaHrxn(T=298K) = -60.653550587927725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7848000e+00 -1.4589000e+00 -3.0035000e-02 /
CHEB / 3.8191000e+00 9.4365000e-01 -3.7054000e-02 /
CHEB / 5.4932000e-01 6.0056000e-01 1.1790000e-02 /
CHEB / -3.7046000e-01 2.1875000e-01 4.5412000e-02 /
CHEB / -3.5037000e-01 -5.3891000e-02 3.9672000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown7(7)       -76.56      102.09      37.21 46.93 55.59 62.99
      74.62 83.21 94.6  null
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!Here are the path reactions and their high-P limit kinetics:
!     C2H5+C4H9O-3=unknown7(7)      1.1500000e+14      -0.35000
0.0000000e+00
!     C4H8-1+C2H5OH=unknown7(7)     1.6297242e+02      2.92024
4.4628571e+04

C2H5+C4H9O-3(+m)=C4H8-1+C2H5OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #16 (unknown7)    deltaHrxn(T=298K) = -65.28278643732911
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3791000e+00 -1.4302000e+00 -3.1990000e-02 /
CHEB / 3.3203000e+00 9.7748000e-01 -3.5971000e-02 /
CHEB / 4.1857000e-01 5.8634000e-01 2.0898000e-02 /
CHEB / -3.4618000e-01 1.7493000e-01 5.4277000e-02 /
CHEB / -3.1086000e-01 -8.8237000e-02 3.8618000e-02 /

!PDepNetwork
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!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown8(8)       -73.53      101.58      37.26 47.66 56.55 63.68
      75.45 83.98 95.43 null
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-1+C2H5OH=unknown8(8)     2.4800000e+01      2.93000
4.3900000e+04
!     C4H8-2+C2H5OH=unknown8(8)     1.1691492e+02      2.87714
4.8857143e+04

C4H8-1+C2H5OH(+m)=C4H8-2+C2H5OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (unknown8)    deltaHrxn(T=298K) = -2.719803185470056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6050000e+01 -1.5432000e+00 -3.1158000e-02 /
CHEB / 2.2509000e+01 8.2556000e-01 -4.7703000e-02 /
CHEB / 1.0433000e+00 5.9591000e-01 -1.2550000e-02 /
CHEB / -2.9263000e-01 3.0978000e-01 2.3422000e-02 /
CHEB / -4.1436000e-01 5.9981000e-02 4.3205000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown9(9)       11.44 103.05      38.31 49.13 57.84 64.32 74.23
      81.41 91.38 null
!     C3H4O       -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04 37.3
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+C4H7-24=unknown9(9)     2.3501400e+11      0.30815
4.9629937e+03
!     C3H5O-enol2+C4H6-13=unknown9(9)     1.1691492e+02      2.87714
4.8857143e+04

C3H5O-enol2+C4H6-13(+m)=C3H4O+C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #41 (unknown9)     deltaHrxn(T=298K) = -
6.989335071390222 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0971000e+00 3.3473000e-08 2.3300000e-08 /
```

```
CHEB / 1.7214000e+01 6.5031000e-08 4.5266000e-08 /
CHEB / 3.3768000e-01 5.9623000e-08 4.1502000e-08 /
CHEB / 1.2455000e-01 5.1559000e-08 3.5889000e-08 /
CHEB / 4.6259000e-02 4.1851000e-08 2.9131000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown10(10)     33.97 91.41 32.54 43.32 52.9  60.77 72.91 81.58
      95.99 null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+C4H8-2=unknown10(10)    6.9200000e+10      0.00000
4.3720000e+04
!     C4H7-24+C3H6=unknown10(10)    6.9200000e+10      0.00000
4.3720000e+04

aC3H5+C4H8-2(+m)=C4H7-24+C3H6(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #94 (unknown10)   deltaHrxn(T=298K) = -0.17986042458998508
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0914000e+01 -6.4634000e-01 -1.9331000e-01 /
CHEB / 1.7898000e+01 7.6789000e-01 1.7881000e-01 /
CHEB / 2.8537000e-01 -1.8784000e-02 7.0113000e-02 /
CHEB / -1.1391000e-01 -9.6689000e-02 -3.6212000e-02 /
CHEB / -1.0423000e-01 -3.0075000e-02 -2.9645000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown12(11)     -52.14      109.83      39.9  50.39 59.58 67.34
      79.47 88.3  99.94 null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+C4H9O-3=unknown12(11)   4.7900000e+14      -0.75000
0.0000000e+00
!     C3H6O-enol2+C4H8-1=unknown12(11)    1.6297242e+02      2.92024
4.4628571e+04
```

```
aC3H5+C4H9O-3(+m)=C3H6O-enol2+C4H8-1(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #107 (unknown12)   deltaHrxn(T=298K) = -
50.58482119489409 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3564000e+00 -1.4393000e+00 -2.7027000e-02 /
CHEB / 5.2731000e+00 9.6938000e-01 -3.0423000e-02 /
CHEB / 5.9012000e-01 5.9722000e-01 1.8191000e-02 /
CHEB / -3.7655000e-01 1.9380000e-01 4.7530000e-02 /
CHEB / -3.2802000e-01 -7.9431000e-02 3.4092000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown13(12)     -47.14      108.93      40.46 51.22 60.49 67.95
      80.26 89.08 102.73      null
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol2+C4H8-1=unknown13(12)    2.4800000e+01      2.93000
4.3900000e+04
!     C3H6O-enol2+C4H8-2=unknown13(12)    1.1691492e+02      2.87714
4.8857143e+04

C3H6O-enol2+C4H8-1(+m)=C3H6O-enol2+C4H8-2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #156 (unknown13)  deltaHrxn(T=298K)
= -2.7198031854700546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6597000e+01 -1.5365000e+00 -2.9526000e-02 /
CHEB / 2.3066000e+01 8.3742000e-01 -4.5202000e-02 /
CHEB / 1.1817000e+00 6.0308000e-01 -1.1869000e-02 /
CHEB / -2.3599000e-01 3.0935000e-01 2.2274000e-02 /
CHEB / -3.9481000e-01 5.0785000e-02 4.1088000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown14(13)     -71.04      127.98      47.96 59.65 69.71 77.7
      90.61 100.25      111.92      null
!     aC3H5       42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76 36.6
!     nSPC(301)         -53.93      102.11      32.84 39.97 46.09 50.94
      58.78 64.89 72.26 null
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
```

```
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+nSPC(301)=unknown14(13) 1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5O2+C4H9O-2=unknown14(13) 6.0300000e+12      0.00000
0.0000000e+00

aC3H5O2+C4H9O-2(+m)=aC3H5+nSPC(301)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #203 (unknown14)   deltaHrxn(T=298K) = -
16.278225283389183 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7990000e+00 -5.8792000e-01 -1.9133000e-01 /
CHEB / 2.1769000e+00 6.9535000e-01 1.9034000e-01 /
CHEB / 4.1633000e-01 -5.6368000e-03 4.9775000e-02 /
CHEB / 6.4862000e-04 -9.9574000e-02 -3.3454000e-02 /
CHEB / -3.2542000e-02 -2.6921000e-02 -2.5295000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown15(14)     -29.46      114.42      41.99 53.25 62.89 70.63
      83.36 92.58 105.02      null
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C3H7O-N1+C4H8-1=unknown15(14) 2.4800000e+01      2.93000
4.3900000e+04
!     C3H7O-N1+C4H8-2=unknown15(14) 1.1691492e+02      2.87714
4.8857143e+04

C3H7O-N1+C4H8-1(+m)=C3H7O-N1+C4H8-2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #275 (unknown15)   deltaHrxn(T=298K) = -
2.7198031854700546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7448000e+01 -1.0098000e+00 -1.4216000e-01 /
CHEB / 2.2331000e+01 1.0424000e+00 5.2675000e-02 /
CHEB / 1.0408000e+00 1.7323000e-01 1.2604000e-01 /
CHEB / 4.2545000e-02 -1.2920000e-01 2.1946000e-02 /
CHEB / -3.4659000e-02 -1.0124000e-01 -4.2419000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown16(15)     -102.36     130.04      50.26 63.04 74.02 82.78
      96.87 107.49      118.87      null
```

```
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     nSPC(301)         -53.93      102.11      32.84 39.97 46.09 50.94
      58.78 64.89 72.26 null
!     C3H7O2      -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67 54.73
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!Here are the path reactions and their high-P limit kinetics:
!     C3H7-1+nSPC(301)=unknown16(15)      1.4157154e+13      -0.15000
2.9166667e+02
!     C3H7O2+C4H9O-2=unknown16(15)  6.0300000e+12      0.00000
0.0000000e+00

C3H7O2+C4H9O-2(+m)=C3H7-1+nSPC(301)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #281 (unknown16)   deltaHrxn(T=298K) = -
0.6399254342064822 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8533000e-01 -9.2512000e-06 -6.4394000e-06 /
CHEB / 4.7286000e+00 1.5084000e-05 1.0500000e-05 /
CHEB / 7.2378000e-01 -7.8610000e-06 -5.4716000e-06 /
CHEB / 6.3613000e-02 2.1503000e-06 1.4967000e-06 /
CHEB / -3.0977000e-02 4.1371000e-08 2.8829000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown17(16)     -83.39      120.42      48.26 61.56 73.05 82.38
      97.59 108.66      123.93      null
!     nC4H10O           -66.09      85.9  27.32 33.59 39.43 44.44 52.4
      58.38 67.83  !MRH
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     nC4H10O+C4H8-1=unknown17(16)  2.4800000e+01      2.93000
4.3900000e+04
!     nC4H10O+C4H8-2=unknown17(16)  1.1691492e+02      2.87714
4.8857143e+04

nC4H10O+C4H8-1(+m)=nC4H10O+C4H8-2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #298 (unknown17)   deltaHrxn(T=298K) = -
2.719803185470051 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6753000e+01 -1.5045000e+00 -1.1887000e-02 /
CHEB / 2.3233000e+01 8.9291000e-01 -1.6814000e-02 /
CHEB / 1.0831000e+00 6.3391000e-01 -9.4623000e-04 /
CHEB / -3.5752000e-01 3.0343000e-01 1.2868000e-02 /
CHEB / -5.0121000e-01 5.8285000e-03 1.6429000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(2)       -37.04      125.55      46.72 58.79 69.56 78.48
      93.24 104.02      119.29      null
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-2+C4H8-1=unknown1(2)    2.4800000e+01      2.93000
4.3900000e+04
!     C4H9O-2+C4H8-2=unknown1(2)    1.1691492e+02      2.87714
4.8857143e+04
!     C4H9O-3+C4H8-1=unknown2(3)    2.4800000e+01      2.93000
4.3900000e+04
!     C4H9O-3+C4H8-2=unknown2(3)    1.1691492e+02      2.87714
4.8857143e+04

C4H9O-2+C4H8-1(+m)=C4H9O-2+C4H8-2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #30 (unknown1)     deltaHrxn(T=298K) = -
2.7198031854700546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7891000e+01 -1.0779000e+00 -1.2863000e-01 /
CHEB / 2.2671000e+01 1.0670000e+00 2.2867000e-02 /
CHEB / 1.0953000e+00 2.2403000e-01 1.2845000e-01 /
CHEB / 4.8958000e-02 -1.1106000e-01 4.1328000e-02 /
CHEB / -4.6204000e-02 -1.0974000e-01 -3.4246000e-02 /

C4H9O-2+C4H8-1(+m)=C4H9O-3+C4H8-2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #30 (unknown1)     deltaHrxn(T=298K) = -
1.5200496304481015 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1460000e+01 -1.6511000e+00 -3.1433000e-01 /
CHEB / 2.4664000e+01 1.7994000e+00 2.1675000e-01 /
CHEB / 1.2773000e+00 1.4508000e-01 1.7520000e-01 /
CHEB / 4.7289000e-02 -2.1110000e-01 -7.5087000e-03 /
CHEB / -4.4404000e-02 -1.1617000e-01 -5.6879000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown3(4)       -29.57      109.91      35.94 44.22 52.03 58.95
      70.08 78.43 89.71 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
```

```
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C4H9O-2           -19.7 88.4  27.35 32.64 37.79 42.3  49.47 54.84
      63.3   !MRH
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     C3H6+C3H7O-N1=unknown3(4)     1.9900000e+03      2.44000
5.3700000e+03
!     C4H9O-2+C2H4=unknown3(4)      1.6297242e+02      2.92024
4.4628571e+04
!     C4H8-1+C2H5O-1=unknown4(5)    1.9900000e+03      2.44000
5.3700000e+03
!     C4H9O-3+C2H4=unknown4(5)      1.6297242e+02      2.92024
4.4628571e+04

C3H6+C3H7O-N1(+m)=C4H9O-2+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #48 (unknown3)    deltaHrxn(T=298K) = -1.419897893608704
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5783000e+00 -8.7685000e-01 -1.7010000e-01 /
CHEB / 1.6731000e+01 9.8090000e-01 1.2352000e-01 /
CHEB / 2.7946000e-01 1.0012000e-01 1.1551000e-01 /
CHEB / -2.5870000e-02 -1.6317000e-01 -2.3105000e-02 /
CHEB / -2.7571000e-02 -1.0679000e-01 -6.4631000e-02 /

C4H8-1+C2H5O-1(+m)=C4H9O-3+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #48 (unknown3)    deltaHrxn(T=298K) = -1.0400243939996923
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4704000e+00 -3.1077000e-01 -1.6822000e-01 /
CHEB / 1.7101000e+01 3.9043000e-01 2.0002000e-01 /
CHEB / 4.9369000e-01 -2.6539000e-02 4.6696000e-03 /
CHEB / 1.4314000e-01 -6.1575000e-02 -3.6626000e-02 /
CHEB / 5.5083000e-02 -1.1150000e-02 -1.3124000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     unknown1(1)       -19.74      105.22      41.07 52.35 61.82 69.02
      80.17 88.4  100.89      null
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
```

```
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C3H5O-enol2+C4H8-1=unknown1(1)      1.1691492e+02      2.87714
4.8857143e+04
!     C3H5O-enol2+C4H8-2=unknown1(1)      1.1691492e+02      2.87714
4.8857143e+04

C3H5O-enol2+C4H8-1(+m)=C3H5O-enol2+C4H8-2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #7 (unknown1)     deltaHrxn(T=298K)
= -2.7198031854700546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0837000e+01 -5.0652000e-03 -3.5063000e-03 /
CHEB / 2.3691000e+01 6.1794000e-03 4.2743000e-03 /
CHEB / 1.6589000e+00 -3.7309000e-04 -2.5405000e-04 /
CHEB / 4.0278000e-01 -8.9263000e-04 -6.1741000e-04 /
CHEB / 9.7363000e-02 1.0245000e-05 5.2319000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3C[OH]CH3       -22.33      74.56 21.77 26.05 29.95 33.3  38.64
      42.68 49.13
!     CH3CH[OH]CH2      -14.14      76.56 22.67 26.97 30.74 33.91 38.93
      42.77 49.05
!     acetone           -51.21      70.9  17.53 21.65 25.52 28.9  34.34
      38.41 44.77
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     H2CCCH3[OH]       -39.44      69.6  20.59 25.3  29.06 32.04 36.55
      39.89 45.32
!Here are the path reactions and their high-P limit kinetics:
!     acetone+H=CH3C[OH]CH3   2.3501400e+11      0.30815
4.9629937e+03
!     H2CCCH3[OH]+H=CH3C[OH]CH3     4.9400000e+13      0.00000
1.5000000e+03
!     CH3CH[OH]CH2=CH3C[OH]CH3      6.2339791e+09      0.93630
3.7689907e+04

acetone+H(+m)=CH3C[OH]CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3C[OH]CH3) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
23.217547267786557 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5905000e+00 5.7155000e-01 -7.1643000e-02 /
CHEB / 4.7657000e-01 8.8161000e-01 -6.0180000e-02 /
CHEB / -7.6590000e-01 4.2962000e-01 3.3478000e-02 /
CHEB / -3.9564000e-01 1.0466000e-01 5.3856000e-02 /
CHEB / -1.6285000e-01 -2.1158000e-02 2.6994000e-02 /
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H2CCCH3[OH]+H(+m)=acetone+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3C[OH]CH3)  deltaHrxn(T=298K) = -11.768418269511542
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2034000e+01 -9.8585000e-01 -1.6888000e-01 /
CHEB / 9.2891000e-01 9.3634000e-01 7.2780000e-02 /
CHEB / -1.8539000e-01 1.9433000e-01 1.0621000e-01 /
CHEB / -1.9971000e-01 -7.3973000e-02 2.5870000e-02 /
CHEB / -8.6973000e-02 -7.4849000e-02 -2.1617000e-02 /

CH3C[OH]CH3(+m)=CH3CH[OH]CH2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3C[OH]CH3)  deltaHrxn(T=298K) = 8.189054151853556
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3528000e+00 1.3091000e+00 -2.2842000e-01 /
CHEB / 1.4564000e+01 6.5874000e-01 1.6785000e-01 /
CHEB / -5.5658000e-01 1.1907000e-01 8.1072000e-02 /
CHEB / -1.9779000e-01 -5.0692000e-02 1.4069000e-03 /
CHEB / -3.7611000e-02 -4.6649000e-02 -2.0259000e-02 /

acetone+H(+m)=CH3CH[OH]CH2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3C[OH]CH3)  deltaHrxn(T=298K) = -15.028493115933001
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4199000e+00 -6.5211000e-01 -2.1715000e-01 /
CHEB / 8.5051000e+00 6.7104000e-01 1.8018000e-01 /
CHEB / -6.5360000e-03 8.7334000e-02 7.3613000e-02 /
CHEB / -1.0187000e-01 -7.2438000e-02 -1.1152000e-02 /
CHEB / -4.7259000e-02 -4.8415000e-02 -2.5700000e-02 /

H2CCCH3[OH]+H(+m)=CH3CH[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH3C[OH]CH3)  deltaHrxn(T=298K) = -26.796911385444545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1792000e+00 -6.2760000e-01 -2.1176000e-01 /
CHEB / 5.1049000e+00 6.6924000e-01 1.8507000e-01 /
CHEB / 1.6983000e-01 6.4494000e-02 6.7459000e-02 /
CHEB / -2.1659000e-02 -8.0147000e-02 -1.7496000e-02 /
CHEB / -8.6048000e-03 -4.4190000e-02 -2.6395000e-02 /

!PDepNetwork acetone && H2CCCH3[OH]
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     acetone           -51.21      70.9  17.53 21.65 25.52 28.9  34.34
      38.41 44.77 Primary Thermo Library: CFG (Species ID: acetone)
!     H2CCCH3[OH]       -39.44      69.6  20.59 25.3  29.06 32.04 36.55
      39.89 45.32 Primary Thermo Library: CFG (Species ID: propen2ol)
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21 Primary Thermo Library: CFG (Species ID: CH3)
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!     C2H3O-2           28.54 64.12 14.36 16.86 18.74 20.19 22.32 23.9
      26.53 Primary Thermo Library: CFG (Species ID: CH2COH)
!     CH2C[OH]CH2       -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26
      40.88 Estimated by Group Additivity
!     H           52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96  4.96
      Primary Thermo Library: CFG (Species ID: H)
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73 Primary Thermo Library: CFG (Species ID: propen1yl)
!     OH          8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23  7.72
      Primary Thermo Library: CFG (Species ID: OH)
!     CH3C[OH]cH        20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23
      39.84 Estimated by Group Additivity
!     CH2C[O]CH3        -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17
      41.25 Primary Thermo Library: CFG (Species ID: propen2oxy)
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
      Primary Thermo Library: CFG (Species ID: acetyl)
!     C2H6              -19.5 54.73 12.57 15.51 18.42 21.06 25.49 28.96
      34.59 Primary Thermo Library: CFG (Species ID: C2H6)
!     CO          -26.44      47.14 6.95  6.99  7.09  7.24  7.57  7.87
      8.34  Primary Thermo Library: CFG (Species ID: CO)
!Here are the path reactions and their high-P limit kinetics:
!     H2CCCH3[OH]=acetone           8.590e+11    0.32        55900.00
!     CH3+C2H3O-2=H2CCCH3[OH] 1.000e+13    0.00        0.00
!     CH2C[OH]CH2+H=H2CCCH3[OH]     5.000e+13    0.00        0.00
!     sC3H5+OH=H2CCCH3[OH]    1.000e+13    0.00        0.00
!     CH3C[OH]cH+H=H2CCCH3[OH]      5.360e+14    0.00        980.00
!     CH2C[O]CH3+H=H2CCCH3[OH]      1.000e+13    0.00        0.00
!     C3H6OJJ(25)=H2CCCH3[OH]       3.980e+07    0.00        0.00
!     CH3+CH3CO=acetone       4.040e+15    -0.80       0.00
!     CH2C[O]CH3+H=acetone          5.000e+13    0.00        0.00
!     C2H6+CO=acetone         5.380e+02    3.29        104500.00

H2CCCH3[OH](+m)=acetone(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
ReactionLibrary: Tautomerization    deltaHrxn(T=298K) = -
11.768418269511542 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -1.0843000e+01 2.2878000e-01 -3.5061000e-02 6.2491000e-04 /
CHEB / 1.6961000e+01 4.2088000e-01 -6.0016000e-02 -3.5880000e-04 /
CHEB / -3.5666000e-01 3.2679000e-01 -3.5671000e-02 -3.6790000e-03 /
CHEB / -2.7005000e-01 2.1232000e-01 -1.0017000e-02 -5.8251000e-03 /

CH3+C2H3O-2(+m)=acetone(+m)                     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -114.98752759228142 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.4880000e+00 2.1405000e+00 -1.0928000e+00 2.1272000e-01 /
CHEB / -1.4898000e+00 2.3898000e+00 -2.0364000e-01 -1.8568000e-01 /
CHEB / -8.6466000e-01 7.6699000e-01 1.5885000e-01 -1.1523000e-01 /
CHEB / -3.9169000e-01 1.8993000e-01 1.2025000e-01 -2.3149000e-02 /

CH3+C2H3O-2(+m)=H2CCCH3[OH](+m)                 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
R_Recombination estimate: (Average:) [ C_methyl , Cd_rad/NonDe ]
      deltaHrxn(T=298K) = -103.21910932276987 kcal/mol
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TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0653000e+01 3.0817000e+00 -1.1026000e+00 2.2933000e-01 /
CHEB / -2.2907000e+00 2.3187000e+00 -2.0626000e-01 -2.1610000e-01 /
CHEB / -1.0670000e+00 7.3942000e-01 1.7536000e-01 -1.2815000e-01 /
CHEB / -4.5507000e-01 1.7825000e-01 1.3906000e-01 -2.6825000e-02 /

CH2C[OH]CH2+H(+m)=acetone(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -100.58898653877529 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1339000e+01 4.8342000e-02 -5.0435000e-01 7.3495000e-02 /
CHEB / -4.5524000e-01 1.8878000e+00 -2.0426000e-01 -1.6119000e-02 /
CHEB / -5.7346000e-01 7.8584000e-01 2.7657000e-02 -5.0964000e-02 /
CHEB / -3.4409000e-01 2.3566000e-01 6.7156000e-02 -2.5866000e-02 /

CH2C[OH]CH2+H(+m)=H2CCCH3[OH](+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/Cd , H_rad ]
      deltaHrxn(T=298K) = -88.82056826926373 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2685000e+01 1.2648000e+00 -4.0749000e-01 8.9137000e-02 /
CHEB / -1.4243000e+00 1.5649000e+00 -2.9359000e-01 -3.0596000e-02 /
CHEB / -8.0585000e-01 7.0685000e-01 1.3599000e-02 -7.3788000e-02 /
CHEB / -3.9475000e-01 2.4009000e-01 8.5461000e-02 -3.7159000e-02 /

CH2C[OH]CH2+H(+m)=CH3+C2H3O-2(+m)         1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = 14.398541053506136
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 7.0209000e+00 -9.2318000e-01 -2.2048000e-01 2.0254000e-02 /
CHEB / 5.7506000e+00 8.1120000e-01 9.6974000e-02 -6.3118000e-02 /
CHEB / 2.2410000e-01 1.8123000e-01 1.1178000e-01 9.8697000e-03 /
CHEB / -2.6922000e-02 -1.7824000e-02 3.3362000e-02 2.5997000e-02 /

sC3H5+OH(+m)=acetone(+m)                   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -121.84704174303755
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 8.8273000e+00 3.2431000e+00 -1.4104000e+00 2.3451000e-01 /
CHEB / -1.9631000e+00 2.5382000e+00 -5.9948000e-02 -3.1169000e-01 /
CHEB / -9.4819000e-01 7.0654000e-01 2.4594000e-01 -1.2871000e-01 /
CHEB / -4.2502000e-01 1.5057000e-01 1.4241000e-01 -1.6165000e-02 /

sC3H5+OH(+m)=H2CCCH3[OH](+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) High-P Limit: R_Recombination estimate:
(Average:) [ Cd_rad/NonDe , O_pri_rad ]   deltaHrxn(T=298K) = -
110.07862347352601 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9761000e+00 4.1543000e+00 -1.4432000e+00 2.3678000e-01 /
CHEB / -2.7480000e+00 2.4966000e+00 -3.9936000e-02 -3.2783000e-01 /
CHEB / -1.1478000e+00 6.8395000e-01 2.6613000e-01 -1.3942000e-01 /
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CHEB / -4.9039000e-01 1.3533000e-01 1.5863000e-01 -2.1289000e-02 /

sC3H5+OH(+m)=CH3+C2H3O-2(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -6.859514150756134
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0711000e+01 -7.9152000e-01 -2.2227000e-01 8.1010000e-03 /
CHEB / 1.5908000e+00 7.6151000e-01 1.3963000e-01 -5.0135000e-02 /
CHEB / 3.4414000e-01 1.1457000e-01 9.9263000e-02 2.4085000e-02 /
CHEB / -8.2955000e-03 -4.1545000e-02 1.0385000e-02 2.2478000e-02 /

sC3H5+OH(+m)=CH2C[OH]CH2+H(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -21.25805520426227
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1078000e+01 -8.0062000e-01 -2.3667000e-01 8.2627000e-03 /
CHEB / 9.5594000e-01 7.2693000e-01 1.4044000e-01 -5.2938000e-02 /
CHEB / 2.3744000e-01 1.4517000e-01 1.0130000e-01 2.0940000e-02 /
CHEB / -1.1744000e-03 -2.3983000e-02 1.9557000e-02 2.3673000e-02 /

CH3C[OH]cH+H(+m)=acetone(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -123.58657544819553 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.7148000e+00 3.6659000e+00 -1.5260000e+00 2.2797000e-01 /
CHEB / -1.7013000e+00 2.5736000e+00 1.0210000e-02 -3.4913000e-01 /
CHEB / -9.7583000e-01 6.7651000e-01 2.7847000e-01 -1.3038000e-01 /
CHEB / -4.2915000e-01 1.3343000e-01 1.4942000e-01 -1.4117000e-02 /

CH3C[OH]cH+H(+m)=H2CCCH3[OH](+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
R_Recombination exact:  [ Cd_pri_rad , H_rad ]  deltaHrxn(T=298K) = -
111.81815717868399 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0862000e+01 4.5733000e+00 -1.5619000e+00 2.2800000e-01 /
CHEB / -2.4843000e+00 2.5357000e+00 3.3286000e-02 -3.6306000e-01 /
CHEB / -1.1750000e+00 6.5474000e-01 2.9931000e-01 -1.4063000e-01 /
CHEB / -4.9483000e-01 1.1763000e-01 1.6516000e-01 -1.9564000e-02 /

CH3C[OH]cH+H(+m)=CH3+C2H3O-2(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -8.599047855914115
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2201000e+01 -7.5636000e-01 -2.2521000e-01 4.3320000e-03 /
CHEB / 1.7402000e+00 7.3342000e-01 1.5074000e-01 -4.5797000e-02 /
CHEB / 3.1769000e-01 1.0654000e-01 9.4016000e-02 2.6150000e-02 /
CHEB / -2.2822000e-03 -4.2595000e-02 6.9028000e-03 2.1025000e-02 /

CH3C[OH]cH+H(+m)=CH2C[OH]CH2+H(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -22.99758890942025 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 4    4 /
CHEB / 1.2437000e+01 -7.5552000e-01 -2.3961000e-01 2.5433000e-03 /
CHEB / 1.2233000e+00 6.9491000e-01 1.5358000e-01 -4.6767000e-02 /
CHEB / 2.0785000e-01 1.3212000e-01 9.6255000e-02 2.4025000e-02 /
CHEB / -1.0445000e-03 -2.6133000e-02 1.4734000e-02 2.2320000e-02 /

CH3C[OH]cH+H(+m)=sC3H5+OH(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -1.739533705157985
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0153000e+01 -7.3098000e-01 -2.2045000e-01 1.9223000e-03 /
CHEB / 2.3375000e+00 7.3109000e-01 1.5576000e-01 -4.2134000e-02 /
CHEB / 3.5738000e-01 8.4293000e-02 8.9757000e-02 2.8727000e-02 /
CHEB / -5.5796000e-03 -4.7910000e-02 6.8391000e-04 1.9140000e-02 /

CH2C[O]CH3+H(+m)=acetone(+m)                    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H2/CO , H_rad ]
      deltaHrxn(T=298K) = -97.1494395308523 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2754000e+01 1.1865000e+00 -3.3846000e-01 5.3845000e-02 /
CHEB / -1.1953000e+00 7.1790000e-01 3.0690000e-02 -3.7763000e-02 /
CHEB / -6.6603000e-01 3.5707000e-01 1.4719000e-02 6.4303000e-04 /
CHEB / -3.2124000e-01 1.1860000e-01 1.6577000e-02 -1.1053000e-03 /

CH2C[O]CH3+H(+m)=H2CCCH3[OH](+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone) High-P Limit:
R_Recombination estimate: (Average:) [ O_rad/OneDe , H_rad ]
      deltaHrxn(T=298K) = -85.38102126134076 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2422000e+01 8.5977000e-01 -2.5731000e-01 5.4982000e-02 /
CHEB / -1.1577000e+00 1.1611000e+00 -2.0467000e-01 -2.1319000e-02 /
CHEB / -6.3421000e-01 5.5844000e-01 1.8402000e-02 -5.8049000e-02 /
CHEB / -3.2719000e-01 1.9701000e-01 7.6515000e-02 -2.9847000e-02 /

CH3+C2H3O-2(+m)=CH2C[O]CH3+H(+m)          1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -17.83808806142911
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0783000e+01 -9.2385000e-01 -2.2452000e-01 2.0606000e-02 /
CHEB / 1.1762000e+00 8.0138000e-01 9.7841000e-02 -6.4328000e-02 /
CHEB / 2.6082000e-01 1.8647000e-01 1.1160000e-01 9.2863000e-03 /
CHEB / 9.1886000e-03 -1.2933000e-02 3.5044000e-02 2.5924000e-02 /

CH2C[OH]CH2+H(+m)=CH2C[O]CH3+H(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -3.4395470079229753 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 9.9141000e+00 -1.1762000e+00 -1.6141000e-01 2.0848000e-02 /
CHEB / 2.4819000e+00 9.3835000e-01 -1.6170000e-02 -4.7266000e-02 /
CHEB / 4.4846000e-01 2.7871000e-01 1.1042000e-01 -2.1110000e-02 /
CHEB / -1.1418000e-03 8.5119000e-03 6.5823000e-02 1.8594000e-02 /
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sC3H5+OH(+m)=CH2C[O]CH3+H(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -24.697602212185238
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.1343000e+01 -7.9611000e-01 -2.4031000e-01 7.4220000e-03 /
CHEB / 7.3597000e-01 7.1642000e-01 1.4222000e-01 -5.3012000e-02 /
CHEB / 1.8155000e-01 1.4773000e-01 1.0146000e-01 2.0957000e-02 /
CHEB / -1.1460000e-02 -2.0399000e-02 2.0677000e-02 2.3800000e-02 /

CH3C[OH]cH+H(+m)=CH2C[O]CH3+H(+m)               1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (acetone)      deltaHrxn(T=298K)
= -26.43713591734322 kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2681000e+01 -7.4979000e-01 -2.4288000e-01 1.3587000e-03 /
CHEB / 1.0175000e+00 6.8443000e-01 1.5542000e-01 -4.6434000e-02 /
CHEB / 1.5355000e-01 1.3403000e-01 9.6411000e-02 2.4164000e-02 /
CHEB / -1.2004000e-02 -2.2989000e-02 1.5682000e-02 2.2490000e-02 /

CH3+CH3CO(+m)=acetone(+m)                 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) High-P Limit: R_Recombination exact:  [
C_methyl , CO_rad/NonDe ]     deltaHrxn(T=298K) = -84.50089408798476
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3065000e+01 3.6197000e-01 -5.5324000e-02 4.0566000e-03 /
CHEB / -1.1118000e+00 5.8155000e-01 -6.1737000e-02 -4.1356000e-03 /
CHEB / -5.7761000e-01 3.3190000e-01 -1.5624000e-03 -9.6142000e-03 /
CHEB / -2.8919000e-01 1.3920000e-01 2.0512000e-02 -4.0455000e-03 /

CH3+CH3CO(+m)=H2CCCH3[OH](+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -72.73247581847323
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.0406000e+01 -1.0962000e+00 -1.3882000e-01 1.0127000e-02 /
CHEB / 5.1311000e-01 1.3958000e+00 -1.4433000e-01 -1.1596000e-02 /
CHEB / -2.5168000e-01 7.1643000e-01 4.3325000e-03 -2.3364000e-02 /
CHEB / -2.9261000e-01 2.5181000e-01 4.5962000e-02 -1.0629000e-02 /

CH3+C2H3O-2(+m)=CH3+CH3CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -30.486633504296652
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2240000e+01 -1.0146000e+00 -3.3563000e-01 -1.2924000e-02 /
CHEB / 5.2658000e-01 8.7431000e-01 1.9827000e-01 -4.1689000e-02 /
CHEB / 1.8330000e-02 2.0553000e-01 1.2506000e-01 1.6336000e-02 /
CHEB / -5.2481000e-02 -8.0574000e-03 3.2266000e-02 2.4769000e-02 /

CH2C[OH]CH2+H(+m)=CH3+CH3CO(+m)           1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -16.088092450790516
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
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CHEB / 1.2197000e+01 -1.7934000e+00 -3.5414000e-01 1.2688000e-02 /
CHEB / 1.3025000e+00 1.4708000e+00 1.3443000e-01 -5.4108000e-02 /
CHEB / 1.5420000e-01 3.6841000e-01 1.3250000e-01 -1.3866000e-02 /
CHEB / -7.1143000e-02 -4.5064000e-03 6.1418000e-02 1.2089000e-02 /

sC3H5+OH(+m)=CH3+CH3CO(+m)          1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (acetone)      deltaHrxn(T=298K) = -37.34614765505278
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.2526000e+01 -7.9077000e-01 -3.0442000e-01 -2.0990000e-02 /
CHEB / 2.3180000e-01 7.0826000e-01 2.0352000e-01 -3.4132000e-02 /
CHEB / -2.8782000e-02 1.5327000e-01 1.1061000e-01 2.9412000e-02 /
CHEB / -7.0637000e-02 -1.3849000e-02 1.9440000e-02 2.4206000e-02 /

CH3C[OH]cH+H(+m)=CH3+CH3CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -39.085681360210764
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3774000e+01 -7.2364000e-01 -2.9417000e-01 -2.5351000e-02 /
CHEB / 5.5871000e-01 6.5991000e-01 2.0683000e-01 -2.8246000e-02 /
CHEB / -4.6163000e-02 1.3595000e-01 1.0363000e-01 3.2520000e-02 /
CHEB / -7.0375000e-02 -1.6786000e-02 1.4484000e-02 2.3403000e-02 /

CH2C[O]CH3+H(+m)=CH3+CH3CO(+m)            1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -12.648545442867539
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 1.3297000e+01 -8.2502000e-01 -2.0549000e-01 1.2431000e-02 /
CHEB / 4.6699000e-01 7.1807000e-01 1.3002000e-01 -3.9687000e-02 /
CHEB / 9.5208000e-02 1.6476000e-01 6.8011000e-02 1.2259000e-02 /
CHEB / -2.2073000e-02 -2.4215000e-02 1.2607000e-02 1.0638000e-02 /

acetone(+m)=C2H6+CO(+m)                   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = 5.269143614421218
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -3.5186000e+01 3.4241000e+00 -4.4477000e-01 -1.0669000e-01 /
CHEB / 3.3418000e+01 6.0313000e-01 -2.0452000e-01 2.2523000e-01 /
CHEB / -6.5729000e-01 2.9758000e-01 -2.6269000e-03 -1.9209000e-02 /
CHEB / -3.2430000e-01 7.9791000e-02 7.8705000e-03 -2.7580000e-02 /

H2CCCH3[OH](+m)=C2H6+CO(+m)               1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -6.499274655090325
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -3.0832000e+01 1.9135000e+00 -9.2190000e-01 1.4070000e-01 /
CHEB / 2.9819000e+01 1.9365000e+00 -1.8573000e-01 -5.2687000e-02 /
CHEB / -6.8105000e-01 6.7610000e-01 1.1337000e-01 -8.9222000e-02 /
CHEB / -3.5200000e-01 1.7190000e-01 1.0143000e-01 -3.5551000e-02 /
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CH3+C2H3O-2(+m)=C2H6+CO(+m)         1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (acetone)      deltaHrxn(T=298K) = -109.7183839778602
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 4.8280000e+00 -1.0208000e+00 -2.7679000e-01 -8.2645000e-03 /
CHEB / 3.4037000e+00 9.3306000e-01 1.6291000e-01 -3.1018000e-02 /
CHEB / 6.5399000e-01 1.6476000e-01 1.0879000e-01 9.7284000e-03 /
CHEB / 9.1786000e-02 -3.0584000e-02 2.4957000e-02 2.2523000e-02 /

CH2C[OH]CH2+H(+m)=C2H6+CO(+m)             1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -95.31984292435406
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 2.9306000e+00 -1.2523000e+00 -3.0877000e-01 -1.2968000e-02 /
CHEB / 5.9855000e+00 1.0780000e+00 1.6096000e-01 -2.3053000e-02 /
CHEB / 5.7287000e-01 2.3568000e-01 1.1374000e-01 -2.5933000e-03 /
CHEB / 6.8140000e-02 -1.8371000e-02 3.8024000e-02 1.8125000e-02 /

sC3H5+OH(+m)=C2H6+CO(+m)            1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (acetone)      deltaHrxn(T=298K) = -116.57789812861634
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 5.5889000e+00 -8.5638000e-01 -2.6524000e-01 -7.5497000e-03 /
CHEB / 2.7453000e+00 7.9171000e-01 1.7186000e-01 -3.5335000e-02 /
CHEB / 5.8924000e-01 1.4157000e-01 1.0175000e-01 2.0885000e-02 /
CHEB / 8.5049000e-02 -3.1749000e-02 1.5261000e-02 2.1624000e-02 /

CH3C[OH]cH+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -118.31743183377432
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 6.9768000e+00 -7.9995000e-01 -2.6132000e-01 -9.3573000e-03 /
CHEB / 2.9773000e+00 7.4509000e-01 1.7657000e-01 -3.3837000e-02 /
CHEB / 5.6130000e-01 1.3081000e-01 9.7438000e-02 2.4275000e-02 /
CHEB / 8.7997000e-02 -3.2184000e-02 1.1550000e-02 2.0746000e-02 /

CH2C[O]CH3+H(+m)=C2H6+CO(+m)              1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (acetone) deltaHrxn(T=298K) = -91.8802959164311
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / 2.8883000e+00 -2.7874000e-01 -1.0964000e-01 -4.4025000e-02 /
CHEB / 6.2900000e+00 2.5150000e-01 9.3815000e-02 4.3695000e-02 /
CHEB / 5.1207000e-01 5.1111000e-02 2.1169000e-02 2.7196000e-03 /
CHEB / 1.4340000e-01 -1.2802000e-02 -3.6822000e-03 -3.7217000e-03 /

CH3+CH3CO(+m)=C2H6+CO(+m)           1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (acetone)      deltaHrxn(T=298K) = -79.23175047356355
kcal/mol
TCHEB / 300.0 2000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 4    4 /
CHEB / -5.0687000e-01 -1.9786000e-01 -1.2519000e-01 -5.3571000e-02 /
CHEB / 8.9583000e+00 1.8486000e-01 1.1472000e-01 4.6099000e-02 /
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CHEB / 2.6487000e-01 4.0516000e-02 2.6555000e-02 1.2861000e-02 /
CHEB / 8.7722000e-02 -1.5044000e-02 -7.7876000e-03 -1.1977000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2C[O]CH3        -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17
      41.25
!     CH3C[OH]cH        20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23
      39.84 null
!     CH2C[OH]CH2       -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26
      40.88 null
!     CH2CO       -10.78      57.63 12.31 14.11 15.57 16.77 18.67 20.12
      22.44
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HCCOH       23.15 59.1  13.44 15.17 16.46 17.47 19.01 20.21 22.29
!     pC3H4             46.16 58.99 14.37 17.14 19.55 21.6  24.93 27.49
      31.65
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+CH3=CH2C[O]CH3    2.8149495e+12      0.00000
7.8566667e+03
!     CH2C[O]CH3=CH3C[OH]cH         8.1282219e+08      1.13906
3.4790987e+04
!     CH3+HCCOH=CH3C[OH]cH    1.9900000e+13      0.00000
1.2100000e+04
!     pC3H4+OH=CH3C[OH]cH     7.6000000e+07      1.70000
1.0000000e+03
!     CH3C[OH]cH=CH2C[OH]CH2        4.5900000e+10      0.97000
3.7700000e+04
!     aC3H4+OH=CH2C[OH]CH2    2.7411173e+10      0.56667
3.7888889e+03
!     CH2C[O]CH3=CH2C[OH]CH2        4.2390000e+09      1.45000
4.2270000e+04
!     sC3H5+O=CH2C[O]CH3      1.0000000e+13      0.00000
0.0000000e+00

CH3C[OH]cH(+m)=CH2C[O]CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -26.437135917343227
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8215000e+00 1.4946000e+00 -2.0500000e-01 /
CHEB / -2.2334000e-01 6.5449000e-01 1.5844000e-01 /
CHEB / -1.7381000e+00 3.9859000e-02 1.9533000e-02 /
CHEB / -8.6167000e-01 -6.6001000e-02 -2.8452000e-02 /
CHEB / -4.0032000e-01 -4.5402000e-02 -1.5818000e-02 /
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CH2C[OH]CH2(+m)=CH2C[O]CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -3.43954700792297
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0746000e+00 1.4629000e+00 -3.3561000e-01 /
CHEB / 1.0667000e+01 9.4672000e-01 1.1667000e-01 /
CHEB / -1.8430000e+00 3.0962000e-01 7.0568000e-02 /
CHEB / -1.0578000e+00 -3.2864000e-02 2.0972000e-02 /
CHEB / -5.3440000e-01 -1.1194000e-01 -1.1477000e-02 /

CH3C[OH]cH(+m)=CH2C[OH]CH2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: intra_H_migration exact:
R3H_DS     Cd_rad_out_singleH     Cs_H_out_2H         deltaHrxn(T=298K)
= -22.99758890942026 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6947000e-01 1.5657000e+00 -3.6334000e-01 /
CHEB / 3.4939000e+00 9.6101000e-01 2.2192000e-01 /
CHEB / -1.5383000e+00 1.6354000e-01 -2.9891000e-03 /
CHEB / -8.7298000e-01 -6.0710000e-02 -7.8283000e-03 /
CHEB / -4.4509000e-01 -8.5133000e-02 -1.3459000e-03 /

CH2CO+CH3(+m)=CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Cd/H2     C_methyl      deltaHrxn(T=298K) = -
30.61633179745659 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0091000e+00 8.1449000e-01 -1.1318000e-01 /
CHEB / 3.7650000e-01 9.0544000e-01 3.4332000e-02 /
CHEB / -1.4156000e+00 3.5124000e-01 5.8454000e-02 /
CHEB / -7.6249000e-01 5.0311000e-02 2.8626000e-02 /
CHEB / -3.9090000e-01 -4.0757000e-02 1.5569000e-04 /

CH3C[OH]cH(+m)=CH2CO+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = 4.179195880113362
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9568000e+00 7.8299000e-01 -1.9358000e-01 /
CHEB / 2.1103000e+00 1.0916000e+00 1.9841000e-01 /
CHEB / -1.3100000e+00 1.8648000e-01 -1.0208000e-02 /
CHEB / -6.8600000e-01 1.4508000e-03 -1.1013000e-02 /
CHEB / -3.4075000e-01 -1.4273000e-02 7.6025000e-03 /

CH2CO+CH3(+m)=CH2C[OH]CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -27.17678478953362
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0413000e+00 -1.5480000e-02 -2.3454000e-01 /
CHEB / 3.0528000e+00 1.7058000e+00 1.3351000e-01 /
CHEB / -1.2984000e+00 4.7092000e-01 9.9207000e-02 /
CHEB / -8.3320000e-01 -2.4861000e-02 3.1738000e-02 /
CHEB / -4.0586000e-01 -9.3360000e-02 -9.1980000e-03 /
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CH3+HCCOH(+m)=CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -64.54275744304203
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9398000e+00 8.2456000e+00 -5.1367000e-01 /
CHEB / 1.1796000e+00 2.2275000e-02 8.7341000e-01 /
CHEB / -1.0118000e+00 -7.8919000e-01 3.8140000e-01 /
CHEB / -4.4640000e-01 -3.9826000e-01 9.4088000e-03 /
CHEB / -3.4691000e-01 -1.1275000e-02 -6.1484000e-02 /

CH3+HCCOH(+m)=CH3C[OH]cH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: R_Addition_MultipleBond
exact:  C_methyl     Ct/Nd_Ct/H           deltaHrxn(T=298K) = -
38.10562152569881 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0348000e+00 7.5465000e+00 7.2516000e-01 /
CHEB / 1.1098000e+00 -2.3219000e-01 8.3193000e-02 /
CHEB / -1.0574000e+00 5.1248000e-03 3.6627000e-02 /
CHEB / -4.3239000e-01 -1.0959000e-01 -1.2038000e-01 /
CHEB / -2.2667000e-01 -1.0926000e-01 -6.2320000e-02 /

CH3+HCCOH(+m)=CH2C[OH]CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -61.10321043511907
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6717000e+00 7.4066000e+00 -7.0137000e-01 /
CHEB / 5.9072000e-02 5.9781000e-01 1.2049000e+00 /
CHEB / -1.3335000e+00 -8.0123000e-01 2.9481000e-01 /
CHEB / -4.5336000e-01 -3.7074000e-01 -7.0323000e-03 /
CHEB / -2.7401000e-01 2.0930000e-02 -4.6086000e-02 /

CH3+HCCOH(+m)=CH2CO+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -33.92642564558545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3914000e+00 -6.3482000e-04 -4.6415000e-04 /
CHEB / 3.9034000e+00 6.5285000e-04 4.4422000e-04 /
CHEB / -8.5746000e-02 2.0146000e-04 1.9198000e-04 /
CHEB / -2.8353000e-02 -1.4584000e-04 -9.7503000e-05 /
CHEB / -2.1815000e-02 -1.3822000e-04 -1.2900000e-04 /

pC3H4+OH(+m)=CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -60.99333197699047
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6199000e+00 5.6862000e+00 -3.0760000e-01 /
CHEB / -1.3605000e+00 2.0717000e-01 1.4601000e-01 /
CHEB / -1.1013000e+00 -1.7004000e-01 2.3674000e-01 /
CHEB / -5.9597000e-01 -1.1679000e-01 4.3041000e-02 /
CHEB / -3.6588000e-01 4.3979000e-03 -5.1721000e-02 /
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pC3H4+OH(+m)=CH3C[OH]cH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ct/Nd_Ct/H     O_pri_rad         deltaHrxn(T=298K)
= -34.556196059647235 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2168000e+00 6.0455000e+00 4.7277000e-01 /
CHEB / -1.5472000e+00 -4.5102000e-01 -5.1568000e-01 /
CHEB / -8.2281000e-01 3.2477000e-02 3.7340000e-02 /
CHEB / -3.9895000e-01 -1.4773000e-02 9.0802000e-02 /
CHEB / -2.5343000e-01 -4.7117000e-02 1.8702000e-02 /

pC3H4+OH(+m)=CH2C[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -57.55378496906749
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2295000e+00 3.9431000e+00 -7.6150000e-01 /
CHEB / -1.8704000e+00 1.7320000e+00 6.4699000e-01 /
CHEB / -1.3331000e+00 -3.4220000e-02 2.9827000e-01 /
CHEB / -6.1965000e-01 -1.9664000e-01 1.5359000e-03 /
CHEB / -3.0552000e-01 -5.0415000e-02 -7.0341000e-02 /

pC3H4+OH(+m)=CH2CO+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -30.377000179533873
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2332000e+01 -3.9454000e-02 -3.1935000e-02 /
CHEB / 9.7515000e-01 4.6788000e-02 3.8042000e-02 /
CHEB / 1.3250000e-01 -2.2654000e-03 -2.1284000e-03 /
CHEB / 3.1146000e-02 -4.4644000e-03 -3.5649000e-03 /
CHEB / -3.6163000e-03 -1.1662000e-03 -8.2644000e-04 /

pC3H4+OH(+m)=CH3+HCCOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = 3.549425466051577
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3921000e+00 -8.5719000e-03 -5.9637000e-03 /
CHEB / 6.1146000e+00 1.1505000e-02 8.0034000e-03 /
CHEB / 3.1502000e-01 -2.7027000e-03 -1.8784000e-03 /
CHEB / 9.7550000e-02 -3.9391000e-04 -2.7530000e-04 /
CHEB / 9.1505000e-03 1.1525000e-04 8.0541000e-05 /

aC3H4+OH(+m)=CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -61.94331068380976
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1535000e+00 5.5499000e+00 -8.4266000e-01 /
CHEB / -2.0285000e+00 1.3592000e+00 9.0810000e-01 /
CHEB / -1.6297000e+00 -3.3078000e-01 3.3337000e-01 /
CHEB / -7.0753000e-01 -2.9599000e-01 -6.7852000e-03 /
CHEB / -3.5948000e-01 -3.9918000e-02 -7.5273000e-02 /
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aC3H4+OH(+m)=CH3C[OH]cH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -35.50617476646653
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.2352000e-01 5.8739000e+00 -7.2358000e-01 /
CHEB / -1.6214000e+00 1.0589000e+00 8.3596000e-01 /
CHEB / -1.3355000e+00 -4.1634000e-01 2.8939000e-01 /
CHEB / -5.3263000e-01 -2.9485000e-01 -1.5677000e-02 /
CHEB / -2.8276000e-01 -2.0357000e-02 -6.7263000e-02 /

aC3H4+OH(+m)=CH2C[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ca_Cd/H2     O_pri_rad           deltaHrxn(T=298K)
= -58.50376367588679 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6347000e+00 5.0324000e+00 -7.2885000e-01 /
CHEB / -3.3400000e+00 1.4438000e+00 8.8668000e-01 /
CHEB / -1.8879000e+00 -2.7888000e-01 3.3138000e-01 /
CHEB / -7.1750000e-01 -2.5415000e-01 -5.2001000e-03 /
CHEB / -3.1725000e-01 -6.0926000e-03 -7.5575000e-02 /

aC3H4+OH(+m)=CH2CO+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -31.326978886353167
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0294000e+01 -3.1815000e-01 -1.7453000e-01 /
CHEB / 1.8042000e+00 4.2317000e-01 2.1837000e-01 /
CHEB / 9.1621000e-03 -7.2135000e-02 -1.4943000e-02 /
CHEB / 1.0155000e-02 -4.9261000e-02 -3.5491000e-02 /
CHEB / 1.7008000e-02 6.0630000e-03 -2.1374000e-03 /

aC3H4+OH(+m)=CH3+HCCOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = 2.5994467592322827
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5395000e+00 -2.2272000e-01 -1.2745000e-01 /
CHEB / 6.4465000e+00 3.0552000e-01 1.6894000e-01 /
CHEB / 4.2710000e-01 -7.1305000e-02 -2.9599000e-02 /
CHEB / 1.2779000e-01 -2.3307000e-02 -1.8842000e-02 /
CHEB / 2.6920000e-02 9.0236000e-03 4.1047000e-03 /

pC3H4+OH(+m)=aC3H4+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = 0.949978706819298
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5827000e+00 -4.0252000e-01 -1.9314000e-01 /
CHEB / 4.5911000e+00 5.3718000e-01 2.4146000e-01 /
CHEB / 6.3894000e-01 -1.0166000e-01 -1.9708000e-02 /
CHEB / 1.7142000e-01 -5.1094000e-02 -3.5488000e-02 /
CHEB / 4.6278000e-02 8.8790000e-03 -7.7083000e-04 /
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sC3H5+O(+m)=CH2C[O]CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3) High-P Limit: Oa_R_Recombination estimate:
(Average:) Cd_rad/NonDe     Oa      deltaHrxn(T=298K) = -
127.73677889873846 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7140000e+01 1.5229000e+01 2.4422000e+00 /
CHEB / -4.6708000e+00 -3.6513000e+00 -1.1980000e-01 /
CHEB / -6.0209000e-01 -4.8625000e-01 -1.0620000e+00 /
CHEB / 7.3089000e-02 1.6827000e-02 -3.3716000e-01 /
CHEB / -1.0497000e-01 -1.9429000e-01 1.5303000e-01 /

sC3H5+O(+m)=CH3C[OH]cH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -101.29964298139524
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9157000e+01 1.2587000e+01 3.5114000e+00 /
CHEB / -4.6318000e+00 -3.3938000e+00 -3.0812000e-01 /
CHEB / -7.7692000e-01 4.7362000e-03 -1.0338000e+00 /
CHEB / -1.0851000e-01 4.3457000e-01 -2.7452000e-01 /
CHEB / -2.0462000e-01 1.1115000e-01 6.6844000e-02 /

sC3H5+O(+m)=CH2C[OH]CH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -124.2972318908155
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5772000e+01 1.4869000e+01 2.4454000e+00 /
CHEB / -5.6536000e+00 -4.1138000e+00 1.3949000e-01 /
CHEB / -8.8809000e-01 -4.0041000e-01 -1.0495000e+00 /
CHEB / -4.8157000e-02 2.3330000e-01 -3.6817000e-01 /
CHEB / -1.3346000e-01 -2.3520000e-02 8.1474000e-02 /

sC3H5+O(+m)=CH2CO+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -97.12044710128188
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3118000e+01 1.1559000e-05 8.0448000e-06 /
CHEB / -1.7940000e-01 -4.1358000e-06 -2.8790000e-06 /
CHEB / -4.7522000e-02 -8.8510000e-07 -6.1430000e-07 /
CHEB / -1.9147000e-02 -1.0569000e-06 -7.3605000e-07 /
CHEB / -1.6057000e-02 -1.0326000e-06 -7.1940000e-07 /

sC3H5+O(+m)=CH3+HCCOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -63.194021455696415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0341000e+01 -2.9474000e-04 -2.0598000e-04 /
CHEB / 8.0749000e-01 2.7963000e-04 1.9589000e-04 /
CHEB / 2.5956000e-01 4.4654000e-05 3.0556000e-05 /
CHEB / 1.0246000e-01 -1.6356000e-05 -1.1275000e-05 /
CHEB / 2.8918000e-02 -1.1112000e-05 -7.7363000e-06 /
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sC3H5+O(+m)=pC3H4+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -66.743446921748
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8103000e+00 6.3092000e-05 4.3399000e-05 /
CHEB / 1.3496000e+00 -8.5019000e-05 -5.8380000e-05 /
CHEB / 3.4579000e-01 3.3401000e-05 2.2888000e-05 /
CHEB / 1.2391000e-01 -6.9087000e-07 -3.9225000e-07 /
CHEB / 3.7901000e-02 -5.4861000e-06 -3.8256000e-06 /

sC3H5+O(+m)=aC3H4+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (CH2C[O]CH3)  deltaHrxn(T=298K) = -65.79346821492871
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0262000e+01 -3.2356000e-03 -2.2725000e-03 /
CHEB / 4.5751000e-01 4.4992000e-03 3.1654000e-03 /
CHEB / 2.1122000e-01 -1.3225000e-03 -9.3928000e-04 /
CHEB / 1.0040000e-01 -1.3194000e-05 -2.7626000e-06 /
CHEB / 2.5513000e-02 7.2990000e-05 4.9864000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C8H17OJ(71)(1)    -39.6 112.16      48.43 61.76 72.69 81.54 95.76
      105.96      121.9 null
!     OC[CH3]3          -23.14      76.55 26.22 32.91 38.66 43.41 50.9
      56.36 64.83 null
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!Here are the path reactions and their high-P limit kinetics:
!     OC[CH3]3+iC4H8=C8H17OJ(71)(1) 1.0000000e+11      0.00000
7.6000000e+03
!     iC4H8+HOC[CH2][CH3]2=C8H17OJ(71)(1) 9.3600000e+01      2.85000
4.1900000e+04

OC[CH3]3+iC4H8(+m)=iC4H8+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C8H17OJ(71))  deltaHrxn(T=298K)
= -1.6002856661875207 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1426000e+00 -4.3156000e-02 -3.4220000e-02 /
CHEB / 1.4100000e+01 6.2801000e-02 4.9285000e-02 /
CHEB / 1.3031000e-01 -1.7966000e-02 -1.3242000e-02 /
CHEB / 4.9685000e-02 -6.6385000e-03 -5.7292000e-03 /
CHEB / 2.0354000e-02 4.6422000e-03 3.4562000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
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```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C7H16O2(67)(2)    -123.47     109.96      46.78 59.68 70.07 78.46
      91.96 101.54      116.42      null
!     CH3C[OH]CH3       -22.33      74.56 21.77 26.05 29.95 33.3  38.64
      42.68 49.13
!     OC[CH3]3          -23.14      76.55 26.22 32.91 38.66 43.41 50.9
      56.36 64.83 null
!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!     tBuOH             -75.1 78.01 27.2  34.21 40.27 45.3  53.28 59.16
      68.42 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3C[OH]CH3+OC[CH3]3=C7H16O2(67)(2) 1.4157154e+13      -0.15000
2.9166667e+02
!     H2CCCH3[OH]+tBuOH=C7H16O2(67)(2)    9.3600000e+01      2.85000
4.1900000e+04

CH3C[OH]CH3+OC[CH3]3(+m)=H2CCCH3[OH]+tBuOH(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H16O2(67))  deltaHrxn(T=298K)
= -69.06295787636385 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1468000e+00 -1.3607000e+00 -4.3212000e-02 /
CHEB / 2.7358000e+00 1.0516000e+00 -4.2159000e-02 /
CHEB / 1.2301000e-01 5.3355000e-01 4.1344000e-02 /
CHEB / -3.8788000e-01 5.6903000e-02 7.7632000e-02 /
CHEB / -2.3142000e-01 -1.6214000e-01 3.9831000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C7H14O(97)(3)     -63.26      104.9 41.52 52.04 61.09 68.55 80.37
      88.99 102.33      null
!     iC4H7             35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62
      50.57
!     CH3C[OH]CH3       -22.33      74.56 21.77 26.05 29.95 33.3  38.64
      42.68 49.13
!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!Here are the path reactions and their high-P limit kinetics:
!     iC4H7+CH3C[OH]CH3=C7H14O(97)(3)     3.5900000e+14      -0.75000
0.0000000e+00
!     HOC[CH2][CH3]2+sC3H5=C7H14O(97)(3)  1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H8+H2CCCH3[OH]=C7H14O(97)(3)     1.6297242e+02      2.92024
4.4628571e+04
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```
HOC[CH2][CH3]2+sC3H5(+m)=iC4H7+CH3C[OH]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6 (C7H14O(97))   deltaHrxn(T=298K)
= -24.347087838070642 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6994000e+00 -1.3756000e+00 -4.7367000e-02 /
CHEB / 1.8223000e+00 1.0262000e+00 -4.5418000e-02 /
CHEB / 1.0906000e-01 5.3139000e-01 4.1649000e-02 /
CHEB / -3.3912000e-01 8.5832000e-02 7.5212000e-02 /
CHEB / -2.4196000e-01 -1.2619000e-01 3.7920000e-02 /

iC4H7+CH3C[OH]CH3(+m)=iC4H8+H2CCCH3[OH](+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6 (C7H14O(97))   deltaHrxn(T=298K)
= -54.52455204860144 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2799000e+00 -1.4595000e+00 -2.9174000e-02 /
CHEB / 4.3706000e+00 9.4383000e-01 -3.5744000e-02 /
CHEB / 5.6284000e-01 6.0323000e-01 1.2193000e-02 /
CHEB / -3.7001000e-01 2.2200000e-01 4.4938000e-02 /
CHEB / -3.4857000e-01 -5.3295000e-02 3.8599000e-02 /

HOC[CH2][CH3]2+sC3H5(+m)=iC4H8+H2CCCH3[OH](+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6 (C7H14O(97))   deltaHrxn(T=298K)
= -78.87163988667209 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4783000e+00 -1.3895000e+00 -4.4325000e-02 /
CHEB / 2.6893000e+00 1.0147000e+00 -4.3868000e-02 /
CHEB / 3.4472000e-01 5.4756000e-01 3.7409000e-02 /
CHEB / -2.3089000e-01 1.0977000e-01 7.2246000e-02 /
CHEB / -2.0573000e-01 -1.1773000e-01 3.9597000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C6H12O2(69)(4)    -92.71      105.56      39.27 49.34 57.47 64.02
      74.55 82.3  93.57 null
!     CH3C[OH]CH3       -22.33      74.56 21.77 26.05 29.95 33.3  38.64
      42.68 49.13
!     CH2C[O]CH3        -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17
      41.25
!     H2CCCH3[OH]             -39.44      69.6  20.59 25.3  29.06 32.04
      36.55 39.89 45.32
!Here are the path reactions and their high-P limit kinetics:
!     CH3C[OH]CH3+CH2C[O]CH3=C6H12O2(69)(4)     1.4157154e+13      -
0.15000      2.9166667e+02
!     H2CCCH3[OH]+H2CCCH3[OH]=C6H12O2(69)(4)    1.1691492e+02
2.87714      4.8857143e+04

CH3C[OH]CH3+CH2C[O]CH3(+m)=H2CCCH3[OH]+H2CCCH3[OH](+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #19 (C6H12O2(69)) deltaHrxn(T=298K)
= -50.39505572404266 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 5.2086000e+00 -1.3640000e+00 -3.7263000e-02 /
CHEB / 5.5060000e+00 1.0402000e+00 -3.4217000e-02 /
CHEB / 5.5034000e-01 5.2393000e-01 3.6931000e-02 /
CHEB / -2.5387000e-01 6.8099000e-02 6.0025000e-02 /
CHEB / -1.6131000e-01 -1.3561000e-01 2.4464000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C7H13OJ(142)(5)   -8.05 95.85 37.47 48.75 58.5  66.29 78.34 86.86
      103.83      null
!     iC4H8             -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34
      54.27
!     CH2C[O]CH3        -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17
      41.25
!     iC4H7             35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62
      50.57
!     acetone           -51.21      70.9  17.53 21.65 25.52 28.9  34.34
      38.41 44.77
!Here are the path reactions and their high-P limit kinetics:
!     iC4H8+CH2C[O]CH3=C7H13OJ(142)(5)    6.9200000e+10      0.00000
4.3720000e+04
!     iC4H7+acetone=C7H13OJ(142)(5) 6.9200000e+10      0.00000
4.3720000e+04

iC4H7+acetone(+m)=iC4H8+CH2C[O]CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #44 (C7H13OJ(142)) deltaHrxn(T=298K) =
7.638921944952764 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0776000e+01 -7.9012000e-01 -1.3849000e-01 /
CHEB / 1.8409000e+01 9.5742000e-01 1.1744000e-01 /
CHEB / -1.0684000e-01 -1.5418000e-02 7.8392000e-02 /
CHEB / -9.8170000e-02 -1.5839000e-01 -3.6002000e-02 /
CHEB / 1.8554000e-04 -4.5428000e-02 -4.0791000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HOCHOOH           -25.83      77.47 18.14 20.12 21.93 23.68 26.4
      28.62 29.35 null
!     HCOOH             -90.87      59.46 11.02 13.15 15.14 16.85 19.42
      21.14 23.32
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     HCOOH+OH=HOCHOOH        2.3501400e+11      0.30815
4.9629937e+03
```

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HOCHOOH(+m)=HCOOH+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6 (CH3O3J) deltaHrxn(T=298K) = -56.3441886673059 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6113000e+00 2.0000000e+00 -3.4952000e-09 /
CHEB / 1.9204000e+00 -9.8453000e-09 -6.8531000e-09 /
CHEB / -1.0897000e+00 -9.2624000e-09 -6.4473000e-09 /
CHEB / -4.7541000e-01 -8.3203000e-09 -5.7915000e-09 /
CHEB / -2.0035000e-01 -7.0601000e-09 -4.9144000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nC3H7OH           -60.69      76.31 20.87 25.94 30.62 34.65 41.04
      45.85 53.48
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H5O-1           -5.79 69.42 16.84 19.49 21.95 24.11 27.6  30.31
      34.79
!     C3H7O-N1          -10.97      79.48 22.04 26.17 30.07 33.41 38.68
      42.66 49.06
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H7O-N2    -13.23      80.42 21.04 25.11 28.98 32.38 37.87 42.05
      48.76
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     HOCHC2H5          -17.02      78.74 21.22 25.67 29.69 33.11 38.51
      42.57 49.06
!     OCH2CH2CH3        -7.25 106.11      21.2  25.72 29.85 33.41 39.13
      43.44 50.19
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C2H5O-1=nC3H7OH     3.3700000e+13      0.00000
0.0000000e+00
!     C3H7O-N1+H=nC3H7OH      1.0000000e+14      0.00000
0.0000000e+00
!     C2H5+CH2OH=nC3H7OH      1.1500000e+13      0.00000
0.0000000e+00
!     C3H7O-N2+H=nC3H7OH      2.0000000e+13      0.00000
0.0000000e+00
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!     C3H7-1+OH=nC3H7OH       7.7000000e+13      0.00000
0.0000000e+00
!     HOCHC2H5+H=nC3H7OH      5.0000000e+13      0.00000
0.0000000e+00
!     OCH2CH2CH3+H=nC3H7OH          1.4157154e+13      -0.15000
2.9166667e+02
!     CH3OH+C2H4=nC3H7OH      1.6297242e+02      2.92024
4.4628571e+04
!     nC3H7OH=C3H6+H2O        3.200e+04    2.53        62940.00

CH3+C2H5O-1(+m)=nC3H7OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination exact:
C_methyl     C_rad/H2/Cs      deltaHrxn(T=298K) = -90.14009864572839
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2469000e+01 6.7569000e-01 -1.4601000e-01 /
CHEB / -2.0512000e+00 1.1214000e+00 -2.1240000e-01 /
CHEB / -1.5426000e+00 6.9295000e-01 -1.0072000e-01 /
CHEB / -9.8265000e-01 3.2777000e-01 -3.5152000e-02 /
CHEB / -5.9675000e-01 1.2013000e-01 -1.5050000e-02 /

C3H7O-N1+H(+m)=nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -101.80881272519659
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2234000e+01 1.4954000e+00 -4.6175000e-01 /
CHEB / -2.8193000e+00 1.3879000e+00 -1.4676000e-01 /
CHEB / -1.8694000e+00 7.0792000e-01 -6.7466000e-02 /
CHEB / -1.1099000e+00 2.8147000e-01 -3.9728000e-02 /
CHEB / -6.3128000e-01 1.0550000e-01 -3.2299000e-02 /

C3H7O-N1+H(+m)=CH3+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -11.66871407946821
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2397000e+01 -8.6905000e-01 -1.7845000e-01 /
CHEB / 1.8082000e-01 8.7522000e-01 1.2170000e-01 /
CHEB / -3.9917000e-01 1.3951000e-01 8.6942000e-02 /
CHEB / -3.6497000e-01 -8.7192000e-02 4.4288000e-03 /
CHEB / -1.6955000e-01 -5.9833000e-02 -2.4526000e-02 /

C2H5+CH2OH(+m)=nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cs     C_rad/H2/O           deltaHrxn(T=298K) = -
86.27088745242834 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2279000e+01 5.4999000e-01 -1.0926000e-01 /
CHEB / -1.9121000e+00 9.6072000e-01 -1.7837000e-01 /
CHEB / -1.4088000e+00 6.4641000e-01 -9.9063000e-02 /
CHEB / -9.4502000e-01 3.3481000e-01 -3.7285000e-02 /
CHEB / -5.8918000e-01 1.2961000e-01 -1.0724000e-02 /
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CH3+C2H5O-1(+m)=C2H5+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -3.8692111933000413
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1523000e+01 -1.2227000e+00 -7.9990000e-02 /
CHEB / 9.2062000e-01 1.0556000e+00 -2.2534000e-02 /
CHEB / -4.2172000e-01 3.2304000e-01 7.9244000e-02 /
CHEB / -4.9558000e-01 -4.3261000e-02 4.9021000e-02 /
CHEB / -2.7223000e-01 -8.6678000e-02 -2.5662000e-03 /

C3H7O-N1+H(+m)=C2H5+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -15.53792527276825
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2915000e+01 -8.8871000e-01 -1.8262000e-01 /
CHEB / -2.7205000e-01 8.7013000e-01 1.1965000e-01 /
CHEB / -5.2828000e-01 1.6359000e-01 8.8546000e-02 /
CHEB / -4.0942000e-01 -7.8248000e-02 9.8443000e-03 /
CHEB / -1.9628000e-01 -6.3099000e-02 -2.2530000e-02 /

C3H7O-N2+H(+m)=nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination exact:
C_rad/H/NonDeC     H_rad      deltaHrxn(T=298K) = -99.54917930602807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1774000e+01 1.2338000e+00 -3.5784000e-01 /
CHEB / -2.7118000e+00 1.3847000e+00 -1.9467000e-01 /
CHEB / -1.8131000e+00 7.1920000e-01 -7.8215000e-02 /
CHEB / -1.0974000e+00 2.9204000e-01 -3.7229000e-02 /
CHEB / -6.3237000e-01 1.0738000e-01 -2.9123000e-02 /

C3H7O-N2+H(+m)=CH3+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -9.409080660299672
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1553000e+01 -9.5417000e-01 -1.5508000e-01 /
CHEB / 3.5865000e-01 9.4564000e-01 8.4158000e-02 /
CHEB / -3.8513000e-01 1.6365000e-01 9.4141000e-02 /
CHEB / -3.9416000e-01 -8.7704000e-02 1.3471000e-02 /
CHEB / -1.9208000e-01 -6.5592000e-02 -2.3461000e-02 /

C3H7O-N1+H(+m)=C3H7O-N2+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -2.259633419168537
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3411000e+00 -7.9071000e-01 -1.7549000e-01 /
CHEB / 1.5342000e+00 8.5320000e-01 1.3498000e-01 /
CHEB / -1.0807000e-01 6.8914000e-02 8.0939000e-02 /
CHEB / -2.6457000e-01 -9.5020000e-02 -1.1350000e-02 /
CHEB / -1.0598000e-01 -4.6556000e-02 -2.6359000e-02 /
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C3H7O-N2+H(+m)=C2H5+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -13.278291853599713
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2111000e+01 -9.8191000e-01 -1.5607000e-01 /
CHEB / -1.2812000e-01 9.4305000e-01 7.8715000e-02 /
CHEB / -5.1226000e-01 1.9269000e-01 9.3854000e-02 /
CHEB / -4.3651000e-01 -7.7151000e-02 2.0000000e-02 /
CHEB / -2.1978000e-01 -6.9167000e-02 -2.0332000e-02 /

C3H7-1+OH(+m)=nC3H7OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     O_pri_rad           deltaHrxn(T=298K) = -
94.57995438134898 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2604000e+01 8.7782000e-01 -2.1672000e-01 /
CHEB / -2.3580000e+00 1.2851000e+00 -2.3168000e-01 /
CHEB / -1.6851000e+00 7.1884000e-01 -9.3070000e-02 /
CHEB / -1.0523000e+00 3.1202000e-01 -3.4363000e-02 /
CHEB / -6.2154000e-01 1.1269000e-01 -2.1902000e-02 /

C3H7-1+OH(+m)=CH3+C2H5O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -4.439855735620597
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1649000e+01 -1.0869000e+00 -1.1408000e-01 /
CHEB / 9.3179000e-01 1.0342000e+00 2.3115000e-02 /
CHEB / -3.5657000e-01 2.1925000e-01 9.7867000e-02 /
CHEB / -4.3692000e-01 -8.0993000e-02 2.9887000e-02 /
CHEB / -2.2345000e-01 -7.6431000e-02 -1.8099000e-02 /

C3H7O-N1+H(+m)=C3H7-1+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -7.228858343847612
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0867000e+01 -8.3942000e-01 -1.7545000e-01 /
CHEB / 5.9916000e-01 8.7357000e-01 1.2577000e-01 /
CHEB / -2.9889000e-01 1.0790000e-01 8.4852000e-02 /
CHEB / -3.3230000e-01 -9.4051000e-02 -2.4027000e-03 /
CHEB / -1.4575000e-01 -5.4158000e-02 -2.6093000e-02 /

C3H7-1+OH(+m)=C2H5+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -8.309066928920638
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2301000e+01 -1.1295000e+00 -1.0798000e-01 /
CHEB / 3.5592000e-01 1.0334000e+00 1.1467000e-02 /
CHEB / -4.7016000e-01 2.5820000e-01 9.2543000e-02 /
CHEB / -4.7540000e-01 -6.5799000e-02 3.7707000e-02 /
CHEB / -2.5355000e-01 -8.0089000e-02 -1.2501000e-02 /
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C3H7O-N2+H(+m)=C3H7-1+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -4.969224924679075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9700000e+00 -9.1357000e-01 -1.5646000e-01 /
CHEB / 8.2819000e-01 9.3858000e-01 9.3130000e-02 /
CHEB / -2.9174000e-01 1.2575000e-01 9.4043000e-02 /
CHEB / -3.6347000e-01 -9.5045000e-02 4.7499000e-03 /
CHEB / -1.6652000e-01 -5.9293000e-02 -2.6062000e-02 /

HOCHC2H5+H(+m)=nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/CsO     H_rad          deltaHrxn(T=298K) = -
95.7595576133711 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2341000e+01 9.1185000e-01 -2.2962000e-01 /
CHEB / -2.3524000e+00 1.3029000e+00 -2.3119000e-01 /
CHEB / -1.6952000e+00 7.2030000e-01 -9.1542000e-02 /
CHEB / -1.0537000e+00 3.0965000e-01 -3.4492000e-02 /
CHEB / -6.1759000e-01 1.1192000e-01 -2.2832000e-02 /

HOCHC2H5+H(+m)=CH3+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -5.619458967642714
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1476000e+01 -1.0729000e+00 -1.1848000e-01 /
CHEB / 9.0413000e-01 1.0265000e+00 2.9407000e-02 /
CHEB / -3.5392000e-01 2.1215000e-01 9.8081000e-02 /
CHEB / -4.2673000e-01 -8.2371000e-02 2.8037000e-02 /
CHEB / -2.1433000e-01 -7.5241000e-02 -1.8938000e-02 /

C3H7O-N1+H(+m)=HOCHC2H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -6.049255111825495
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1926000e+00 -8.3469000e-01 -1.7521000e-01 /
CHEB / 1.2130000e+00 8.7248000e-01 1.2652000e-01 /
CHEB / -1.4117000e-01 1.0338000e-01 8.4512000e-02 /
CHEB / -2.7732000e-01 -9.4602000e-02 -3.3878000e-03 /
CHEB / -1.2258000e-01 -5.3282000e-02 -2.6225000e-02 /

HOCHC2H5+H(+m)=C2H5+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -9.488670160942755
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2117000e+01 -1.1143000e+00 -1.1293000e-01 /
CHEB / 3.3974000e-01 1.0265000e+00 1.7957000e-02 /
CHEB / -4.6929000e-01 2.4969000e-01 9.3587000e-02 /
CHEB / -4.6588000e-01 -6.7890000e-02 3.5805000e-02 /
CHEB / -2.4406000e-01 -7.8897000e-02 -1.3669000e-02 /
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C3H7O-N2+H(+m)=HOCHC2H5+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -3.789621692656958
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2857000e+00 -9.0557000e-01 -1.5783000e-01 /
CHEB / 1.4535000e+00 9.3399000e-01 9.6118000e-02 /
CHEB / -1.3738000e-01 1.2139000e-01 9.3329000e-02 /
CHEB / -3.0808000e-01 -9.5576000e-02 3.4876000e-03 /
CHEB / -1.4310000e-01 -5.8494000e-02 -2.6209000e-02 /

HOCHC2H5+H(+m)=C3H7-1+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -1.1796032320221173
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7809000e+00 -1.0101000e+00 -1.3098000e-01 /
CHEB / 1.4958000e+00 1.0064000e+00 5.0835000e-02 /
CHEB / -2.8986000e-01 1.6525000e-01 1.0109000e-01 /
CHEB / -3.9530000e-01 -9.1708000e-02 1.6568000e-02 /
CHEB / -1.8583000e-01 -6.8444000e-02 -2.3456000e-02 /

OCH2CH2CH3+H(+m)=nC3H7OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
105.52856630668373 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0366000e+01 2.0903000e+00 -6.7217000e-01 /
CHEB / -3.0388000e+00 1.3214000e+00 -3.8069000e-02 /
CHEB / -1.9949000e+00 6.6740000e-01 -4.2241000e-02 /
CHEB / -1.1679000e+00 2.6137000e-01 -4.2970000e-02 /
CHEB / -6.5217000e-01 1.0317000e-01 -3.6147000e-02 /

CH3+C2H5O-1(+m)=OCH2CH2CH3+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 15.388467660955335
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9277000e+00 -7.0694000e-01 -2.0759000e-01 /
CHEB / 5.4228000e+00 7.3015000e-01 1.7625000e-01 /
CHEB / -2.6353000e-01 1.0176000e-01 7.0121000e-02 /
CHEB / -2.6090000e-01 -8.1769000e-02 -1.0020000e-02 /
CHEB / -1.1554000e-01 -4.9361000e-02 -2.4159000e-02 /

C3H7O-N1+H(+m)=OCH2CH2CH3+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 3.719753581487126
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1680000e+01 -6.5005000e-01 -1.9107000e-01 /
CHEB / 2.7640000e+00 7.2530000e-01 1.7646000e-01 /
CHEB / -2.3422000e-02 3.4919000e-02 5.7331000e-02 /
CHEB / -1.9258000e-01 -8.9522000e-02 -2.1987000e-02 /
CHEB / -6.6442000e-02 -3.4661000e-02 -2.3016000e-02 /
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C2H5+CH2OH(+m)=OCH2CH2CH3+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 19.25767885425538
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5673000e+00 -7.1424000e-01 -2.1444000e-01 /
CHEB / 6.4709000e+00 7.2076000e-01 1.7785000e-01 /
CHEB / -3.5764000e-01 1.1826000e-01 7.3569000e-02 /
CHEB / -3.1160000e-01 -7.5159000e-02 -6.4333000e-03 /
CHEB / -1.4376000e-01 -5.2035000e-02 -2.3666000e-02 /

C3H7O-N2+H(+m)=OCH2CH2CH3+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 5.979387000655663
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0600000e+01 -6.6962000e-01 -1.9383000e-01 /
CHEB / 3.2061000e+00 7.3449000e-01 1.7505000e-01 /
CHEB / -7.2978000e-02 5.1004000e-02 6.0878000e-02 /
CHEB / -2.1656000e-01 -9.0382000e-02 -1.9169000e-02 /
CHEB / -8.3750000e-02 -3.8381000e-02 -2.3778000e-02 /

C3H7-1+OH(+m)=OCH2CH2CH3+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 10.948611925334738
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0231000e+01 -6.9358000e-01 -2.0061000e-01 /
CHEB / 4.2964000e+00 7.3652000e-01 1.7507000e-01 /
CHEB / -1.7313000e-01 7.9700000e-02 6.6061000e-02 /
CHEB / -2.4810000e-01 -8.7571000e-02 -1.4203000e-02 /
CHEB / -1.0595000e-01 -4.4902000e-02 -2.4312000e-02 /

HOCHC2H5+H(+m)=OCH2CH2CH3+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = 9.769008693312621
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0116000e+01 -6.9115000e-01 -1.9982000e-01 /
CHEB / 4.2059000e+00 7.3666000e-01 1.7510000e-01 /
CHEB / -1.5430000e-01 7.6566000e-02 6.5452000e-02 /
CHEB / -2.3958000e-01 -8.8141000e-02 -1.4781000e-02 /
CHEB / -9.7789000e-02 -4.4210000e-02 -2.4287000e-02 /

CH3OH+C2H4(+m)=nC3H7OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: 1,3_Insertion_ROR estimate:
(Average:) CH3OH     Cd/unsub_Cd/unsub          deltaHrxn(T=298K) = -
25.767403352486298 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3982000e+00 3.0454000e-01 -5.0602000e-02 /
CHEB / 1.5253000e+01 5.6282000e-01 -9.0606000e-02 /
CHEB / -6.2697000e-01 4.4164000e-01 -6.3949000e-02 /
CHEB / -6.2205000e-01 2.8836000e-01 -3.3097000e-02 /
CHEB / -4.7465000e-01 1.4871000e-01 -9.1006000e-03 /
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CH3+C2H5O-1(+m)=CH3OH+C2H4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -64.37269529324209
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0138000e+01 -1.3272000e+00 -6.9302000e-02 /
CHEB / 7.6759000e-01 9.9733000e-01 -4.3280000e-02 /
CHEB / -3.9256000e-01 4.1090000e-01 5.2366000e-02 /
CHEB / -4.6722000e-01 3.4128000e-02 5.5206000e-02 /
CHEB / -3.0012000e-01 -7.0886000e-02 1.6760000e-02 /

C3H7O-N1+H(+m)=CH3OH+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -76.04140937271029
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0963000e+01 -9.2103000e-01 -2.0134000e-01 /
CHEB / -1.6122000e-02 8.3940000e-01 1.1797000e-01 /
CHEB / -5.4071000e-01 2.1324000e-01 9.3612000e-02 /
CHEB / -4.2414000e-01 -4.8011000e-02 2.4000000e-02 /
CHEB / -2.2861000e-01 -6.4076000e-02 -1.4704000e-02 /

C2H5+CH2OH(+m)=CH3OH+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -60.50348409994205
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5507000e+00 -1.3964000e+00 -5.4007000e-02 /
CHEB / 1.0446000e+00 9.5902000e-01 -5.2949000e-02 /
CHEB / -2.9573000e-01 4.6027000e-01 2.9186000e-02 /
CHEB / -4.9590000e-01 8.0503000e-02 5.0691000e-02 /
CHEB / -3.3286000e-01 -5.9484000e-02 2.4950000e-02 /

C3H7O-N2+H(+m)=CH3OH+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -73.78177595354175
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0257000e+01 -1.0355000e+00 -1.6651000e-01 /
CHEB / 6.7103000e-02 9.1630000e-01 6.8142000e-02 /
CHEB / -5.2570000e-01 2.5317000e-01 9.3410000e-02 /
CHEB / -4.4536000e-01 -3.9839000e-02 3.5701000e-02 /
CHEB / -2.5163000e-01 -6.8773000e-02 -9.0833000e-03 /

C3H7-1+OH(+m)=CH3OH+C2H4(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -68.81255102886269
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0664000e+01 -1.2163000e+00 -1.0359000e-01 /
CHEB / 4.0521000e-01 9.9935000e-01 -1.0127000e-02 /
CHEB / -4.7489000e-01 3.3736000e-01 7.8137000e-02 /
CHEB / -4.6863000e-01 -9.5968000e-03 5.1554000e-02 /
CHEB / -2.8335000e-01 -7.4087000e-02 4.5341000e-03 /
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HOCHC2H5+H(+m)=CH3OH+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -69.9921542608848
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0451000e+01 -1.1980000e+00 -1.0986000e-01 /
CHEB / 4.0929000e-01 9.9466000e-01 -3.1173000e-03 /
CHEB / -4.7604000e-01 3.2693000e-01 8.0975000e-02 /
CHEB / -4.6141000e-01 -1.4332000e-02 5.0282000e-02 /
CHEB / -2.7414000e-01 -7.3841000e-02 2.8097000e-03 /

OCH2CH2CH3+H(+m)=CH3OH+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -79.76116295419742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6046000e+00 -7.1331000e-01 -2.3910000e-01 /
CHEB / -1.8406000e-01 6.8134000e-01 1.8600000e-01 /
CHEB / -5.9271000e-01 1.5053000e-01 8.3828000e-02 /
CHEB / -4.2262000e-01 -5.4614000e-02 3.7110000e-03 /
CHEB / -2.1006000e-01 -5.4452000e-02 -2.0844000e-02 /

nC3H7OH(+m)=C3H6+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH) High-P Limit: 1,3_Insertion_ROR Primary
Kinetic Library: Mike   deltaHrxn(T=298K) = 8.468763178519012 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4618000e+01 2.3288000e-01 -3.5802000e-02 /
CHEB / 2.1498000e+01 4.3569000e-01 -6.5099000e-02 /
CHEB / -4.9664000e-01 3.5490000e-01 -4.8116000e-02 /
CHEB / -5.3536000e-01 2.4748000e-01 -2.6886000e-02 /
CHEB / -4.2755000e-01 1.4201000e-01 -8.1726000e-03 /

CH3+C2H5O-1(+m)=C3H6+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -81.67133546720937
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9277000e+00 -1.3585000e+00 -6.9226000e-02 /
CHEB / 1.1870000e+00 9.7034000e-01 -5.0665000e-02 /
CHEB / -2.9522000e-01 4.3090000e-01 4.3100000e-02 /
CHEB / -4.2325000e-01 6.2588000e-02 5.4635000e-02 /
CHEB / -2.8961000e-01 -5.8838000e-02 2.2483000e-02 /

C3H7O-N1+H(+m)=C3H6+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -93.34004954667758
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0567000e+01 -9.2446000e-01 -2.1175000e-01 /
CHEB / 4.8614000e-01 8.2554000e-01 1.1834000e-01 /
CHEB / -4.4906000e-01 2.2624000e-01 9.6354000e-02 /
CHEB / -3.9957000e-01 -3.7082000e-02 2.9769000e-02 /
CHEB / -2.2906000e-01 -6.2672000e-02 -1.0775000e-02 /
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C2H5+CH2OH(+m)=C3H6+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -77.80212427390933
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4280000e+00 -1.4311000e+00 -5.3810000e-02 /
CHEB / 1.4068000e+00 9.2203000e-01 -5.9031000e-02 /
CHEB / -1.9222000e-01 4.7520000e-01 1.8257000e-02 /
CHEB / -4.3937000e-01 1.1280000e-01 4.6273000e-02 /
CHEB / -3.1733000e-01 -4.1768000e-02 2.8694000e-02 /

C3H7O-N2+H(+m)=C3H6+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -91.08041612750904
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8964000e+00 -1.0481000e+00 -1.7329000e-01 /
CHEB / 5.5555000e-01 9.0415000e-01 6.4384000e-02 /
CHEB / -4.3435000e-01 2.6978000e-01 9.3660000e-02 /
CHEB / -4.1802000e-01 -2.5774000e-02 4.1621000e-02 /
CHEB / -2.5035000e-01 -6.6186000e-02 -3.8134000e-03 /

C3H7-1+OH(+m)=C3H6+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -86.11119120282997
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0376000e+01 -1.2416000e+00 -1.0506000e-01 /
CHEB / 8.6379000e-01 9.8275000e-01 -1.7958000e-02 /
CHEB / -3.8202000e-01 3.5844000e-01 7.2757000e-02 /
CHEB / -4.3431000e-01 1.2143000e-02 5.5125000e-02 /
CHEB / -2.7774000e-01 -6.7533000e-02 1.1085000e-02 /

HOCHC2H5+H(+m)=C3H6+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -87.29079443485209
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0154000e+01 -1.2222000e+00 -1.1173000e-01 /
CHEB / 8.7191000e-01 9.7912000e-01 -1.0784000e-02 /
CHEB / -3.8354000e-01 3.4776000e-01 7.6238000e-02 /
CHEB / -4.2810000e-01 6.4291000e-03 5.4303000e-02 /
CHEB / -2.6911000e-01 -6.7899000e-02 9.3328000e-03 /

OCH2CH2CH3+H(+m)=C3H6+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -97.0598031281647
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1497000e+00 -7.0195000e-01 -2.5208000e-01 /
CHEB / 3.4006000e-01 6.6266000e-01 1.9151000e-01 /
CHEB / -4.9972000e-01 1.5741000e-01 8.8740000e-02 /
CHEB / -4.0166000e-01 -4.7900000e-02 7.9682000e-03 /
CHEB / -2.1217000e-01 -5.4517000e-02 -1.9223000e-02 /
```

```
CH3OH+C2H4(+m)=C3H6+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #101 (nC3H7OH)    deltaHrxn(T=298K) = -17.29864017396728
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2647000e+01 -1.5757000e+00 -4.0004000e-02 /
CHEB / 1.9414000e+01 7.4588000e-01 -6.2056000e-02 /
CHEB / 6.4360000e-01 4.9565000e-01 -2.2088000e-02 /
CHEB / -2.7930000e-01 2.2575000e-01 1.2020000e-02 /
CHEB / -3.2858000e-01 4.0582000e-02 2.3526000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     iC4H7OJ(30) -10.03      77.94 24.19 29.26 33.77 37.63 43.83 48.46
      55.63 null
!     iC4H7OJ(48) -2.2  83.37 23.03 28.2  33.04 36.99 43.43 48.09 53.71
      null
!     iC4H7OJ(51) -14.3 80.77 22.74 28.03 33.0  37.03 43.54 48.2  52.91
      null
!     iC4H7OJ(17) -2.16 80.25 24.19 29.61 34.26 38.15 44.29 48.75 55.48
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     C3H7-1            23.67 69.29 17.11 21.27 25.14 28.53 33.95 38.14
      44.75 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C3H4O-enone       -15.03      68.27 16.5  19.56 22.34 24.77 28.73
      31.72 36.36 null
!     C3H7-2            21.02 69.01 16.58 20.27 24.03 27.49 33.13 37.52
      44.42 null
```

```
!     HCC[CH3]2   55.3  72.75 21.39 25.9  29.94 33.42 39.09 43.4  50.18
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     aC3H4            46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     CH2OH            -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!Here are the path reactions and their high-P limit kinetics:
!     C3H3OH+CH3=iC4H7OJ(15)  1.5800000e+11      0.00000
4.9700000e+03
!     C4H6Oi-13+H=iC4H7OJ(15) 2.3501400e+11      0.30815
4.9629937e+03
!     tSPC(110)+H=iC4H7OJ(15) 1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7OJ(30)=iC4H7OJ(15) 1.4106558e+11      0.61833
2.7168333e+04
!     C4H6Oi-12+H=iC4H7OJ(30) 5.2263889e+12      0.04600
5.0666667e+03
!     C4H6Oi-13+H=iC4H7OJ(30) 2.1300000e+13      0.00000
5.0000000e+02
!     tSPC(110)+H=iC4H7OJ(30) 5.0000000e+13      0.00000
0.0000000e+00
!     iC4H7OJ(48)=iC4H7OJ(30) 6.2339791e+09      0.93630
3.7689907e+04
!     C3H6+HCO=iC4H7OJ(48)    5.200e+11    0.00        8560.00
!     C3H4O+CH3=iC4H7OJ(48)   2.4300000e+12      0.00000
1.0200000e+04
!     C4H6Oi-13+H=iC4H7OJ(48) 9.3000000e+12      0.00000
5.2000000e+03
!     tSPC(110)+H=iC4H7OJ(48) 1.4157154e+13      -0.15000
2.9166667e+02
!     C3H7-1+CO=iC4H7OJ(48)   5.9198482e+04      2.36750
7.2970000e+04
!     iC4H7OJ=iC4H7OJ(51)     2.0320555e+08      1.13906
3.4790987e+04
!     CH3+C3H4O-enone=iC4H7OJ(51)   9.2300000e+12      0.00000
9.4000000e+03
!     C4H6Oi-12+H=iC4H7OJ(51) 1.8833259e+13      0.00000
2.9000000e+03
!     iC4H7OJ(30)=iC4H7OJ(51) 2.0320555e+08      1.13906
3.4790987e+04
!     C3H7-2+CO=iC4H7OJ(51)   8.610e+07    1.36        4800.00
!     HCC[CH3]2+O=iC4H7OJ(30) 1.0000000e+13      0.00000
0.0000000e+00
!     iC4H7OJ(17)=iC4H7OJ(15) 2.1620731e+09      0.93000
3.2050000e+04
!     aC3H4+CH2OH=iC4H7OJ(17) 1.9263655e+11      0.04067
9.2900000e+03
!     C4H7OJ(79)=iC4H7OJ(17)  9.0000000e+11      0.00000
2.9400000e+04
!     C4H7OJ(79)=iC4H7OJ(15)  8.1282219e+08      1.13906
3.4790987e+04

iC4H7OJ(30)(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: intra_H_migration estimate:
```

```
(Average:) R4H_SDS     O_rad_out     Cs_H_out_2H      deltaHrxn(T=298K)
= 0.19992958701252483 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0165000e-01 7.9178000e-01 -8.6347000e-02 /
CHEB / 7.8675000e+00 1.2295000e+00 -7.4646000e-02 /
CHEB / -9.7129000e-01 6.1478000e-01 3.3558000e-02 /
CHEB / -5.0422000e-01 1.9786000e-01 4.4850000e-02 /
CHEB / -2.2509000e-01 4.2276000e-02 1.1957000e-02 /

iC4H7OJ(15)(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 7.629409838638563
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.6801000e+00 1.5526000e+00 -3.8630000e-01 /
CHEB / 1.4368000e+01 1.3645000e+00 1.7593000e-01 /
CHEB / -9.0864000e-01 4.7411000e-01 3.7647000e-02 /
CHEB / -4.1039000e-01 1.0629000e-01 -6.2266000e-03 /
CHEB / -1.5341000e-01 1.8591000e-02 5.5826000e-03 /

iC4H7OJ(30)(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 7.829339425651088
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0472000e+00 2.2283000e+00 -1.5838000e-01 /
CHEB / 1.3720000e+01 7.6802000e-01 2.2083000e-02 /
CHEB / -9.4036000e-01 3.7143000e-01 -2.6989000e-02 /
CHEB / -3.5108000e-01 1.4878000e-01 -8.6664000e-03 /
CHEB / -1.3198000e-01 6.0289000e-02 1.9549000e-02 /

iC4H7OJ(15)(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -4.4693535008429315
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8617000e+00 1.3683000e+00 -2.2284000e-01 /
CHEB / 1.1579000e+01 1.4728000e+00 3.7320000e-03 /
CHEB / -6.5645000e-01 5.3801000e-01 6.6480000e-02 /
CHEB / -3.5845000e-01 1.4527000e-01 1.1829000e-02 /
CHEB / -1.1678000e-01 3.4954000e-02 -7.8454000e-03 /

iC4H7OJ(30)(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    Others-C_rad_out_Cs2    CO_H_out
      deltaHrxn(T=298K) = -4.269423913830407 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8471000e+00 2.3665000e+00 -4.8171000e-02 /
CHEB / 1.0506000e+01 5.6934000e-01 -5.2648000e-02 /
CHEB / -6.9416000e-01 3.6916000e-01 -3.3384000e-02 /
CHEB / -2.6118000e-01 2.1030000e-01 -1.2527000e-02 /
CHEB / -7.9331000e-02 1.0137000e-01 8.5618000e-03 /

iC4H7OJ(48)(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: intra_H_migration estimate:
```

```
(Average:) Others-R3H_SS    C_rad_out_2H     CO_H_out
      deltaHrxn(T=298K) = -12.098763339481494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.6138000e+00 3.6873000e+00 -1.5118000e-01 /
CHEB / 1.0157000e+01 2.4785000e-01 1.3999000e-01 /
CHEB / -6.2834000e-01 2.9009000e-02 2.1506000e-02 /
CHEB / -2.4575000e-02 -2.5288000e-02 -2.0497000e-02 /
CHEB / 1.0746000e-01 -2.9832000e-04 -1.3800000e-02 /

iC4H7OJ(17)(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: intra_H_migration estimate:
(Average:) R3H_SS_2Cd     C_rad_out_2H     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -7.669293892204099 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0722000e+00 8.4760000e-01 -1.2946000e-01 /
CHEB / 1.0000000e+01 9.3360000e-01 -4.9308000e-02 /
CHEB / -7.9023000e-01 6.8420000e-01 -6.7667000e-02 /
CHEB / -5.0436000e-01 3.6372000e-01 3.1069000e-03 /
CHEB / -2.5427000e-01 1.1955000e-01 4.4415000e-02 /

iC4H7OJ(17)(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -7.869223479216624
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5931000e+00 -1.0327000e-01 -2.9634000e-01 /
CHEB / 1.0444000e+01 1.8791000e+00 2.1803000e-02 /
CHEB / -8.1516000e-01 8.1437000e-01 3.9634000e-02 /
CHEB / -5.8851000e-01 2.6227000e-01 1.8124000e-02 /
CHEB / -2.9737000e-01 5.3050000e-02 1.5741000e-02 /

iC4H7OJ(17)(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -0.03988405356553537
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7610000e+00 2.4311000e-01 -4.1728000e-01 /
CHEB / 1.3846000e+01 2.2284000e+00 8.5523000e-02 /
CHEB / -5.5537000e-01 8.3425000e-01 2.1566000e-02 /
CHEB / -4.8432000e-01 1.8516000e-01 4.2141000e-02 /
CHEB / -2.0793000e-01 -2.2550000e-02 4.5640000e-02 /

iC4H7OJ(17)(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -12.13864739304703
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0080000e+01 2.1834000e-01 -3.2134000e-01 /
CHEB / 1.2422000e+01 2.2006000e+00 4.4456000e-03 /
CHEB / -4.5356000e-01 8.8428000e-01 3.8769000e-02 /
CHEB / -4.9004000e-01 2.3191000e-01 3.6178000e-02 /
CHEB / -1.8850000e-01 -6.8050000e-03 3.5771000e-02 /

C3H3OH+CH3(+m)=iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
```

```
exact:  Ca_Cd/H2     C_methyl       deltaHrxn(T=298K) = -
49.22467114910896 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3080000e+00 8.1993000e-01 -6.6330000e-02 /
CHEB / 6.6807000e-01 6.6470000e-01 -9.6673000e-02 /
CHEB / -6.1874000e-01 3.9991000e-01 7.7171000e-03 /
CHEB / -2.5000000e-01 1.0151000e-01 7.3575000e-02 /
CHEB / -8.2671000e-02 -2.8744000e-02 4.8226000e-02 /

C3H3OH+CH3(+m)=iC4H7OJ(30)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -49.424600736121484
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1853000e+00 2.3284000e-01 -2.7622000e-01 /
CHEB / 6.9004000e-01 1.3091000e+00 9.1964000e-02 /
CHEB / -6.7389000e-01 4.2456000e-01 6.5168000e-02 /
CHEB / -2.9933000e-01 2.1997000e-02 4.8973000e-02 /
CHEB / -1.0903000e-01 -6.0846000e-02 2.4340000e-02 /

C3H3OH+CH3(+m)=iC4H7OJ(48)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -41.59526131047039
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6574000e+00 2.7624000e-01 -2.8861000e-01 /
CHEB / 2.8634000e+00 1.3968000e+00 1.2905000e-01 /
CHEB / -1.4116000e-01 3.8662000e-01 7.1894000e-02 /
CHEB / -1.5846000e-01 -2.3098000e-02 4.7951000e-02 /
CHEB / -5.3832000e-02 -7.9349000e-02 1.8705000e-02 /

C3H3OH+CH3(+m)=iC4H7OJ(51)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -53.694024649951885
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7531000e+00 3.0548000e-01 -2.6633000e-01 /
CHEB / 2.2647000e+00 1.3693000e+00 1.0763000e-01 /
CHEB / -2.1657000e-01 3.9899000e-01 7.5855000e-02 /
CHEB / -1.3867000e-01 -1.8706000e-02 5.1301000e-02 /
CHEB / -7.1172000e-03 -8.3836000e-02 1.8204000e-02 /

C3H3OH+CH3(+m)=iC4H7OJ(17)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -41.55537725690486
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5087000e+00 -4.6014000e-01 -1.7090000e-01 /
CHEB / 1.9809000e+00 1.6682000e+00 -1.6016000e-01 /
CHEB / -4.6612000e-01 7.4660000e-01 8.5352000e-02 /
CHEB / -3.5469000e-01 7.6579000e-02 1.4604000e-01 /
CHEB / -1.3689000e-01 -1.2288000e-01 5.6962000e-02 /

C4H6Oi-13+H(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
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exact:  Cd/H2_Cd/Nd/De     H_rad          deltaHrxn(T=298K) = -
31.686210542619634 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2717000e+01 4.0874000e-01 -5.0147000e-02 /
CHEB / -6.7216000e-01 6.4114000e-01 -5.7295000e-02 /
CHEB / -5.5544000e-01 4.1092000e-01 -3.0709000e-02 /
CHEB / -2.8115000e-01 2.2138000e-01 -4.5520000e-03 /
CHEB / -1.3576000e-01 9.2247000e-02 1.7568000e-02 /

C4H6Oi-13+H(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
exact:  Cd/Nd/De_Cd/H2     H_rad          deltaHrxn(T=298K) = -
23.85687111696855 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3132000e+00 1.4107000e+00 -2.0829000e-01 /
CHEB / 4.0619000e-01 4.2073000e-01 1.6238000e-01 /
CHEB / -4.6167000e-01 4.0164000e-02 2.7419000e-02 /
CHEB / 5.9865000e-03 -3.8737000e-02 -2.6874000e-02 /
CHEB / 7.4951000e-02 1.4265000e-02 -2.0358000e-02 /

C4H6Oi-13+H(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -35.95563445645004
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6548000e+00 5.1919000e-01 -5.8371000e-02 /
CHEB / 2.2365000e+00 7.9300000e-01 -6.6243000e-02 /
CHEB / -6.6984000e-02 4.5846000e-01 -1.7779000e-02 /
CHEB / -1.3069000e-01 1.8144000e-01 2.9745000e-02 /
CHEB / -2.8575000e-02 2.2495000e-02 4.5318000e-02 /

C4H6Oi-13+H(+m)=C3H3OH+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 17.738390193501843
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7440000e+00 -1.6357000e+00 -2.4017000e-01 /
CHEB / 7.5108000e+00 1.3486000e+00 8.5947000e-02 /
CHEB / -3.0393000e-01 3.9702000e-01 8.5283000e-02 /
CHEB / -2.8648000e-01 -3.1544000e-02 5.3435000e-02 /
CHEB / -1.2827000e-01 -9.3028000e-02 1.4609000e-02 /

tSPC(110)+H(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
85.09080982060031 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2319000e+01 1.3587000e+00 -2.1994000e-01 /
CHEB / -1.4395000e+00 6.2751000e-01 1.6618000e-01 /
CHEB / -5.2733000e-01 8.2560000e-02 6.9404000e-02 /
CHEB / -9.3434000e-02 -5.3965000e-02 -2.8378000e-03 /
CHEB / 2.8292000e-03 -3.0843000e-02 -1.6503000e-02 /
```

```
tSPC(110)+H(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Recombination estimate:
(Average:) Y_rad     H_rad          deltaHrxn(T=298K) = -
77.26147039494923 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1226000e+00 1.7986000e+00 -3.6033000e-02 /
CHEB / -2.0249000e-01 1.2432000e-01 -2.1047000e-02 /
CHEB / -8.8217000e-02 9.0980000e-02 4.3569000e-02 /
CHEB / 8.1094000e-02 6.8141000e-03 2.3396000e-02 /
CHEB / 5.9350000e-02 -1.9707000e-02 -4.2881000e-03 /

tSPC(110)+H(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -89.36023373443072
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7888000e+00 1.3706000e+00 -2.1615000e-01 /
CHEB / -2.7183000e-01 6.3236000e-01 1.7091000e-01 /
CHEB / -1.8815000e-01 7.5429000e-02 6.8040000e-02 /
CHEB / 4.9993000e-02 -5.9456000e-02 -6.3230000e-03 /
CHEB / 1.0176000e-01 -3.2848000e-02 -1.8630000e-02 /

tSPC(110)+H(+m)=C3H3OH+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -35.666209084478844
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3063000e+01 -6.7145000e-01 -2.4988000e-01 /
CHEB / 6.9356000e-02 7.0356000e-01 2.1809000e-01 /
CHEB / -1.4925000e-01 6.4171000e-02 6.9031000e-02 /
CHEB / -1.0801000e-01 -7.9278000e-02 -1.9839000e-02 /
CHEB / -4.2913000e-02 -3.8180000e-02 -2.4374000e-02 /

C4H6Oi-12+H(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -37.02189413782108
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5256000e+00 -1.1719000e-01 -2.8257000e-01 /
CHEB / 1.5055000e+00 1.4002000e+00 8.9891000e-02 /
CHEB / -5.8763000e-01 5.0047000e-01 4.8010000e-02 /
CHEB / -3.6092000e-01 9.9555000e-02 2.4225000e-02 /
CHEB / -1.4872000e-01 -2.0352000e-02 2.2237000e-02 /

C4H6Oi-12+H(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_O     H_rad       deltaHrxn(T=298K) = -
37.221823724833605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0264000e+01 5.2227000e-01 -6.1148000e-02 /
CHEB / 6.3436000e-01 7.7235000e-01 -8.1395000e-02 /
CHEB / -6.4074000e-01 4.3352000e-01 -1.6835000e-02 /
CHEB / -2.9134000e-01 1.6480000e-01 3.6355000e-02 /
CHEB / -1.1918000e-01 2.4376000e-02 4.5636000e-02 /
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C4H6Oi-12+H(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.39248429918252
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8901000e+00 5.0559000e-01 -1.2679000e-01 /
CHEB / 3.5829000e+00 9.9113000e-01 -8.5517000e-03 /
CHEB / -1.2412000e-01 4.1474000e-01 8.9030000e-04 /
CHEB / -1.4531000e-01 9.4415000e-02 5.1443000e-02 /
CHEB / -5.4383000e-02 -2.4724000e-02 4.8962000e-02 /

C4H6Oi-12+H(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/Nd2_Ck     H_rad        deltaHrxn(T=298K) = -
41.491247638664014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4876000e+00 1.9975000e+00 -2.7260000e-04 /
CHEB / -9.1749000e-02 -2.0720000e-03 2.7305000e-04 /
CHEB / -2.5928000e-01 -1.0164000e-04 -7.0446000e-04 /
CHEB / 6.7956000e-02 1.6587000e-03 -7.3202000e-04 /
CHEB / 1.0314000e-01 1.7616000e-03 -1.6036000e-04 /

C4H6Oi-12+H(+m)=iC4H7OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.352600245616983
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0429000e+00 -1.3905000e+00 -3.4705000e-01 /
CHEB / 3.5274000e+00 2.3287000e+00 1.9205000e-02 /
CHEB / -4.2835000e-01 8.6166000e-01 6.8483000e-02 /
CHEB / -4.8830000e-01 1.1846000e-01 8.3937000e-02 /
CHEB / -2.0814000e-01 -1.0161000e-01 5.3587000e-02 /

C4H6Oi-12+H(+m)=C3H3OH+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 12.202777011287871
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9039000e+00 -1.6099000e+00 -2.5617000e-01 /
CHEB / 6.2278000e+00 1.4113000e+00 1.2143000e-01 /
CHEB / -1.2080000e-01 3.4885000e-01 8.5620000e-02 /
CHEB / -2.5913000e-01 -6.4713000e-02 4.9770000e-02 /
CHEB / -1.2704000e-01 -1.0023000e-01 7.2216000e-03 /

C4H6Oi-12+H(+m)=C4H6Oi-13+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -5.535613182213972
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7167000e+00 -1.3773000e+00 -6.2725000e-02 /
CHEB / 1.2432000e+00 9.0822000e-01 -7.2041000e-02 /
CHEB / -5.0428000e-01 4.4527000e-01 1.4401000e-02 /
CHEB / -3.7594000e-01 9.8776000e-02 6.4192000e-02 /
CHEB / -1.8111000e-01 -4.4286000e-02 4.9385000e-02 /
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tSPC(110)+H(+m)=C4H6Oi-12+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -47.86898609576671
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2504000e+00 -6.1546000e-01 -2.1196000e-01 /
CHEB / -1.8689000e+00 6.3617000e-01 1.7570000e-01 /
CHEB / -5.8399000e-01 6.5776000e-02 6.5711000e-02 /
CHEB / -2.0016000e-01 -6.5893000e-02 -1.0657000e-02 /
CHEB / -6.6414000e-02 -3.4421000e-02 -2.0789000e-02 /

iC4H7OJ(15)(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 24.877522583789617
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7618000e+00 -2.5200000e-01 -3.6163000e-01 /
CHEB / 1.5264000e+01 1.5369000e+00 1.8219000e-01 /
CHEB / -7.0124000e-01 4.8820000e-01 3.7485000e-02 /
CHEB / -4.6390000e-01 7.7760000e-02 9.7089000e-03 /
CHEB / -2.0064000e-01 -1.8709000e-02 2.1394000e-02 /

iC4H7OJ(30)(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 25.077452170802143
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1649000e+00 3.6590000e-01 -1.4920000e-01 /
CHEB / 1.4627000e+01 9.3355000e-01 1.6894000e-02 /
CHEB / -6.9437000e-01 4.2473000e-01 -1.9108000e-02 /
CHEB / -3.8654000e-01 1.3920000e-01 1.9102000e-02 /
CHEB / -1.7542000e-01 2.3365000e-02 4.1712000e-02 /

C3H6+HCO(+m)=iC4H7OJ(48)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
Primary Kinetic Library: Mike       deltaHrxn(T=298K) = -
17.248112745151055 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8242000e+00 1.0512000e+00 -1.6204000e-01 /
CHEB / 1.2617000e+00 8.3041000e-01 1.0286000e-01 /
CHEB / -7.7346000e-01 2.1557000e-01 6.0041000e-02 /
CHEB / -1.9391000e-01 -3.5799000e-02 1.1678000e-02 /
CHEB / 5.1709000e-03 -5.0740000e-02 -8.5824000e-03 /

C3H6+HCO(+m)=iC4H7OJ(51)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.346876084632548
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4134000e+00 1.7372000e+00 -1.2580000e-01 /
CHEB / 6.1447000e+00 2.4118000e-01 1.3784000e-01 /
CHEB / 4.2591000e-02 2.2068000e-03 -8.7590000e-04 /
CHEB / 1.2091000e-01 -1.6979000e-02 -2.6877000e-02 /
CHEB / 1.2273000e-01 1.4535000e-02 -7.0201000e-03 /
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```
iC4H7OJ(17)(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 17.208228691585518
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6175000e+00 -1.4941000e+00 -4.0156000e-01 /
CHEB / 1.4736000e+01 2.4321000e+00 8.6403000e-02 /
CHEB / -4.7207000e-01 8.3156000e-01 4.9234000e-02 /
CHEB / -5.8128000e-01 1.1103000e-01 7.5693000e-02 /
CHEB / -2.5602000e-01 -9.3410000e-02 5.5172000e-02 /

C3H3OH+CH3(+m)=C3H6+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -24.347148565319337
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4573000e+00 -1.6419000e+00 -2.7531000e-01 /
CHEB / 3.6788000e+00 1.4406000e+00 1.4243000e-01 /
CHEB / 1.1117000e-02 3.4436000e-01 8.0663000e-02 /
CHEB / -2.4244000e-01 -6.5490000e-02 4.7390000e-02 /
CHEB / -1.2131000e-01 -9.7471000e-02 8.6908000e-03 /

C4H6Oi-13+H(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -6.608758371817494
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0649000e+01 -4.7237000e-01 -1.6727000e-01 /
CHEB / 2.1105000e+00 3.6672000e-01 1.6027000e-01 /
CHEB / 6.7280000e-02 -1.6396000e-02 -1.1548000e-02 /
CHEB / 1.5321000e-02 1.4725000e-02 -3.8799000e-02 /
CHEB / -1.1930000e-02 6.9248000e-02 -3.2002000e-03 /

tSPC(110)+H(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -60.01335764979818
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2865000e+01 -1.9692000e-01 -3.5118000e-02 /
CHEB / 1.3921000e-01 1.3072000e-01 -1.7032000e-02 /
CHEB / -3.1717000e-02 9.0429000e-02 4.5306000e-02 /
CHEB / -1.1804000e-02 1.0392000e-03 2.0834000e-02 /
CHEB / -1.2033000e-02 -2.3827000e-02 -7.4610000e-03 /

C4H6Oi-12+H(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -12.144371554031466
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2900000e+00 -1.4050000e+00 -1.1573000e-01 /
CHEB / 4.6663000e+00 1.0544000e+00 -7.6966000e-03 /
CHEB / 7.7600000e-02 3.9705000e-01 2.1956000e-02 /
CHEB / -2.0653000e-01 4.1576000e-02 6.6758000e-02 /
CHEB / -1.1130000e-01 -6.5549000e-02 4.2784000e-02 /
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iC4H7OJ(15)(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 24.31728330443804
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9848000e+00 -2.4501000e-01 -3.6067000e-01 /
CHEB / 1.5731000e+01 1.5400000e+00 1.8201000e-01 /
CHEB / -5.7731000e-01 4.8664000e-01 3.7489000e-02 /
CHEB / -4.2107000e-01 7.6026000e-02 1.0442000e-02 /
CHEB / -1.8342000e-01 -2.0203000e-02 2.1885000e-02 /

iC4H7OJ(30)(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 24.517212891450562
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3895000e+00 3.7046000e-01 -1.4873000e-01 /
CHEB / 1.5095000e+01 9.3729000e-01 1.6437000e-02 /
CHEB / -5.6888000e-01 4.2479000e-01 -1.8755000e-02 /
CHEB / -3.4333000e-01 1.3780000e-01 2.0232000e-02 /
CHEB / -1.5824000e-01 2.1611000e-02 4.2324000e-02 /

C3H4O+CH3(+m)=iC4H7OJ(48)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H/De_Cd/H2     C_methyl        deltaHrxn(T=298K) = -
16.687873465799477 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8356000e+00 1.0875000e+00 -1.6296000e-01 /
CHEB / 1.7902000e+00 8.2742000e-01 1.0382000e-01 /
CHEB / -7.3725000e-01 1.8585000e-01 6.2413000e-02 /
CHEB / -1.5216000e-01 -4.6270000e-02 1.0310000e-02 /
CHEB / 2.6372000e-02 -4.9990000e-02 -9.5239000e-03 /

C3H4O+CH3(+m)=iC4H7OJ(51)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -28.78663680528097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2529000e+00 1.7401000e+00 -1.2441000e-01 /
CHEB / 6.5505000e+00 2.3913000e-01 1.3705000e-01 /
CHEB / 7.2173000e-02 9.8188000e-04 -1.8502000e-03 /
CHEB / 1.5066000e-01 -1.6065000e-02 -2.6774000e-02 /
CHEB / 1.3978000e-01 1.5078000e-02 -6.5963000e-03 /

iC4H7OJ(17)(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 16.64798941223394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8313000e+00 -1.4853000e+00 -4.0107000e-01 /
CHEB / 1.5200000e+01 2.4359000e+00 8.6152000e-02 /
CHEB / -3.5301000e-01 8.2969000e-01 5.0388000e-02 /
CHEB / -5.3911000e-01 1.0781000e-01 7.6835000e-02 /
CHEB / -2.3847000e-01 -9.5698000e-02 5.5237000e-02 /
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C4H6Oi-13+H(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -7.168997651169072
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0400000e+01 -4.6729000e-01 -1.6523000e-01 /
CHEB / 2.6144000e+00 3.6279000e-01 1.5933000e-01 /
CHEB / 1.9899000e-01 -1.9038000e-02 -1.3381000e-02 /
CHEB / 5.5261000e-02 1.8241000e-02 -3.8497000e-02 /
CHEB / 2.2702000e-03 7.0913000e-02 -1.9911000e-03 /

tSPC(110)+H(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -60.57359692914975
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2702000e+01 -1.9681000e-01 -3.5101000e-02 /
CHEB / 5.7656000e-01 1.3088000e-01 -1.6927000e-02 /
CHEB / 8.6578000e-02 9.0395000e-02 4.5346000e-02 /
CHEB / 3.0128000e-02 8.6988000e-04 2.0755000e-02 /
CHEB / 4.4506000e-03 -2.3930000e-02 -7.5469000e-03 /

C4H6Oi-12+H(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -12.704610833383043
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0846000e+00 -1.4022000e+00 -1.1538000e-01 /
CHEB / 5.1336000e+00 1.0555000e+00 -7.9074000e-03 /
CHEB / 1.9937000e-01 3.9599000e-01 2.2669000e-02 /
CHEB / -1.6426000e-01 3.9789000e-02 6.7129000e-02 /
CHEB / -9.4539000e-02 -6.6568000e-02 4.2401000e-02 /

iC4H7OJ(15)(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 7.079267960171265
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3428000e+01 1.0645000e+00 -2.9741000e-01 /
CHEB / 2.7813000e+01 8.9676000e-01 2.1667000e-01 /
CHEB / -2.5552000e-01 1.2780000e-01 8.9490000e-02 /
CHEB / -1.1407000e-01 -7.2419000e-02 1.6108000e-03 /
CHEB / -2.9609000e-02 -4.8098000e-02 -2.0271000e-02 /

iC4H7OJ(30)(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 7.279197547183784
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3116000e+01 1.2059000e+00 -2.1131000e-01 /
CHEB / 2.7589000e+01 7.4845000e-01 1.2816000e-01 /
CHEB / -1.7020000e-01 1.2831000e-01 8.7631000e-02 /
CHEB / -3.7524000e-02 -5.5940000e-02 1.2218000e-02 /
CHEB / -2.4065000e-03 -4.2498000e-02 -1.6307000e-02 /
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iC4H7OJ(48)(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -0.5501418784673007
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9716000e+01 1.9968000e+00 -2.2364000e-03 /
CHEB / 2.4446000e+01 2.8238000e-03 1.9630000e-03 /
CHEB / -9.9733000e-02 2.6026000e-04 1.8007000e-04 /
CHEB / 6.8128000e-02 -4.9957000e-04 -3.4890000e-04 /
CHEB / 6.1234000e-02 -1.3943000e-04 -9.8512000e-05 /

iC4H7OJ(51)(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 11.548621461014193
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9867000e+01 1.9477000e+00 -3.5799000e-04 /
CHEB / 2.9931000e+01 3.2105000e-02 -1.1995000e-02 /
CHEB / 3.1955000e-01 2.3491000e-02 5.8932000e-03 /
CHEB / 2.3411000e-01 1.7981000e-03 7.5483000e-03 /
CHEB / 1.6378000e-01 -3.5233000e-03 1.1648000e-03 /

iC4H7OJ(17)(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -0.5900259320328374
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1832000e+01 2.3810000e-01 -5.1316000e-01 /
CHEB / 2.5819000e+01 1.6676000e+00 3.4234000e-01 /
CHEB / -2.0761000e-01 2.6443000e-01 1.7884000e-01 /
CHEB / -1.7687000e-01 -1.3464000e-01 1.2037000e-02 /
CHEB / -5.6599000e-02 -1.0159000e-01 -4.0470000e-02 /

C4H6Oi-13+H(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -24.40701299543585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.1443000e+00 -2.9932000e-01 -1.6446000e-02 /
CHEB / 1.7235000e+01 2.2902000e-01 -4.9485000e-02 /
CHEB / 2.7981000e-01 1.0531000e-01 5.1148000e-02 /
CHEB / 1.2057000e-01 -5.7517000e-03 2.9936000e-02 /
CHEB / 4.7795000e-02 -2.5443000e-02 -4.6642000e-03 /

tSPC(110)+H(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -77.81161227341653
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1376000e+00 -1.8346000e-01 -3.8287000e-02 /
CHEB / 3.7548000e+00 1.5250000e-01 4.3788000e-04 /
CHEB / 1.1172000e+00 7.5336000e-02 4.8570000e-02 /
CHEB / 3.3236000e-01 -2.5265000e-02 5.6708000e-03 /
CHEB / 9.3609000e-02 -2.7617000e-02 -1.6246000e-02 /
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C4H6Oi-12+H(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.94262617764982
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7762000e+00 -7.5758000e-01 -2.0282000e-01 /
CHEB / 1.5857000e+01 7.6409000e-01 1.4234000e-01 /
CHEB / 3.8898000e-01 1.0308000e-01 8.5305000e-02 /
CHEB / 1.0866000e-01 -7.6660000e-02 9.6180000e-04 /
CHEB / 3.3764000e-02 -4.7991000e-02 -2.3741000e-02 /

C3H6+HCO(+m)=C3H7-1+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -17.798254623618355
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1614000e+01 -3.1028000e-03 -2.1528000e-03 /
CHEB / 1.9587000e+01 2.8807000e-03 2.0015000e-03 /
CHEB / 2.2055000e-01 2.3230000e-04 1.6033000e-04 /
CHEB / 9.1050000e-02 -4.9884000e-04 -3.4815000e-04 /
CHEB / 3.7599000e-02 -1.2899000e-04 -9.0707000e-05 /

CH3+C3H4O-enone(+m)=iC4H7OJ(15)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.609825918764585
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5799000e-01 -1.0516000e-01 -2.6702000e-01 /
CHEB / 5.8029000e+00 1.5666000e+00 9.3850000e-02 /
CHEB / 1.2432000e-01 4.9231000e-01 6.2449000e-02 /
CHEB / -1.6129000e-01 5.7317000e-02 2.8097000e-02 /
CHEB / -7.8409000e-02 -5.4498000e-02 2.4668000e-02 /

CH3+C3H4O-enone(+m)=iC4H7OJ(30)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.80975550577711
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3094000e-01 5.7107000e-01 -6.0465000e-02 /
CHEB / 4.8599000e+00 8.5256000e-01 -7.0436000e-02 /
CHEB / 1.1589000e-01 4.5761000e-01 -4.5105000e-03 /
CHEB / -7.0019000e-02 1.4219000e-01 4.8285000e-02 /
CHEB / -4.5924000e-02 -1.3148000e-02 5.1069000e-02 /

CH3+C3H4O-enone(+m)=iC4H7OJ(48)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -21.980416080126023
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5248000e+00 1.7886000e+00 -1.0047000e-01 /
CHEB / 5.9218000e+00 2.0111000e-01 1.2044000e-01 /
CHEB / 5.1285000e-01 -1.3366000e-02 -1.6303000e-02 /
CHEB / 2.6570000e-01 1.6665000e-03 -2.2014000e-02 /
CHEB / 1.2887000e-01 1.9771000e-02 1.0725000e-03 /

CH3+C3H4O-enone(+m)=iC4H7OJ(51)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) C_methyl     Cd/H/Nd_Ck          deltaHrxn(T=298K)
= -34.07917941960751 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4952000e+00 1.9994000e+00 -4.3089000e-04 /
CHEB / 2.1074000e+00 7.2664000e-04 5.0550000e-04 /
CHEB / -2.8236000e-01 -5.2970000e-05 -3.6784000e-05 /
CHEB / 4.9542000e-02 -8.1913000e-05 -5.6998000e-05 /
CHEB / 9.1436000e-02 -1.5233000e-05 -1.0613000e-05 /

CH3+C3H4O-enone(+m)=iC4H7OJ(17)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -21.940532026560486
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1306000e+00 -1.3043000e+00 -3.3659000e-01 /
CHEB / 8.0793000e+00 2.4768000e+00 3.4485000e-02 /
CHEB / 1.4210000e-01 8.3277000e-01 8.7863000e-02 /
CHEB / -3.2861000e-01 5.4961000e-02 9.4364000e-02 /
CHEB / -1.3285000e-01 -1.4472000e-01 5.2260000e-02 /

C4H6Oi-13+H(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -1.8764550368425237
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8638000e+00 -1.3372000e+00 -6.1936000e-02 /
CHEB / 5.6035000e+00 9.6205000e-01 -6.2745000e-02 /
CHEB / 4.3416000e-01 4.3812000e-01 2.5945000e-02 /
CHEB / -8.1350000e-02 5.8156000e-02 7.1019000e-02 /
CHEB / -5.3668000e-02 -7.7136000e-02 4.4970000e-02 /

tSPC(110)+H(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -55.28105431482321
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0368000e+01 -6.0572000e-01 -2.0911000e-01 /
CHEB / 6.7568000e-01 6.3805000e-01 1.7878000e-01 /
CHEB / 1.7792000e-01 5.8206000e-02 6.3603000e-02 /
CHEB / 8.6417000e-02 -7.0447000e-02 -1.3846000e-02 /
CHEB / 4.8310000e-02 -3.5025000e-02 -2.2080000e-02 /

C4H6Oi-12+H(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -7.412068219056495
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1459000e+00 -2.3185000e-03 -1.1179000e-04 /
CHEB / 2.8348000e+00 -1.2655000e-03 1.6966000e-04 /
CHEB / 5.7341000e-01 1.3721000e-03 -7.9833000e-04 /
CHEB / 1.5166000e-01 2.2554000e-03 -2.8752000e-04 /
CHEB / 2.7439000e-02 9.2956000e-04 5.2009000e-04 /

CH3+C3H4O-enone(+m)=C3H6+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -4.732303334974969
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3152000e-01 -1.6793000e-01 -7.7887000e-02 /
CHEB / 7.3503000e+00 1.6255000e-01 1.0091000e-01 /
CHEB / 8.1366000e-01 -1.4463000e-02 -2.6056000e-02 /
CHEB / 2.0191000e-01 1.5254000e-02 -1.4260000e-02 /
CHEB / 4.6701000e-02 1.5651000e-02 9.1421000e-03 /

CH3+C3H4O-enone(+m)=C3H4O+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -5.292542614326543
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.4599000e-01 -1.6596000e-01 -7.6862000e-02 /
CHEB / 7.8318000e+00 1.6024000e-01 9.9794000e-02 /
CHEB / 9.3649000e-01 -1.4035000e-02 -2.6238000e-02 /
CHEB / 2.4324000e-01 1.5675000e-02 -1.3928000e-02 /
CHEB / 6.2445000e-02 1.5355000e-02 9.3723000e-03 /

iC4H7OJ(15)(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 4.4295805765524925
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.2881000e+00 -5.4466000e-01 -2.2544000e-01 /
CHEB / 1.2494000e+01 1.5563000e+00 1.2516000e-02 /
CHEB / -4.6799000e-01 5.5393000e-01 6.9533000e-02 /
CHEB / -4.2649000e-01 1.3896000e-01 1.2054000e-02 /
CHEB / -2.1319000e-01 2.0803000e-02 -3.1121000e-03 /

iC4H7OJ(30)(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 4.6295101635650155
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3117000e+00 4.1431000e-01 -5.1326000e-02 /
CHEB / 1.1435000e+01 6.4799000e-01 -5.6832000e-02 /
CHEB / -4.7591000e-01 4.1301000e-01 -3.1142000e-02 /
CHEB / -3.2017000e-01 2.1970000e-01 -3.3100000e-03 /
CHEB / -1.7477000e-01 8.9173000e-02 1.9232000e-02 /

iC4H7OJ(48)(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -3.1998292620860695
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9075000e+00 1.7005000e+00 -1.4467000e-01 /
CHEB / 1.0992000e+01 2.5179000e-01 1.4160000e-01 /
CHEB / -3.8569000e-01 2.4458000e-02 1.6356000e-02 /
CHEB / -4.4687000e-02 -2.3983000e-02 -2.3338000e-02 /
CHEB / 3.2843000e-02 3.6036000e-03 -1.2870000e-02 /

iC4H7OJ(51)(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 8.898934077395424
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 6.2043000e+00 1.7478000e+00 -1.2112000e-01 /
CHEB / 2.3150000e+00 3.0289000e-01 1.4098000e-01 /
CHEB / -8.0230000e-01 -1.4107000e-02 -6.7153000e-04 /
CHEB / -6.0103000e-02 -3.5288000e-02 -1.7037000e-02 /
CHEB / 1.1866000e-01 -9.1632000e-03 -5.8006000e-03 /

iC4H7OJ(17)(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -3.2397133156516063
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3224000e+00 -1.6833000e+00 -3.2233000e-01 /
CHEB / 1.3258000e+01 2.3013000e+00 9.6920000e-03 /
CHEB / -3.2211000e-01 9.0131000e-01 4.7043000e-02 /
CHEB / -5.7703000e-01 2.0930000e-01 4.6791000e-02 /
CHEB / -2.8436000e-01 -3.5732000e-02 4.2403000e-02 /

C3H3OH+CH3(+m)=C3H7-2+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -44.79509057255646
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7987000e+00 -1.6659000e+00 -2.6176000e-01 /
CHEB / 3.0616000e+00 1.3916000e+00 1.1455000e-01 /
CHEB / -4.2862000e-02 3.8698000e-01 7.9913000e-02 /
CHEB / -2.0953000e-01 -3.5993000e-02 5.1090000e-02 /
CHEB / -1.0681000e-01 -9.2980000e-02 1.4570000e-02 /

C4H6Oi-13+H(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -27.056700379054618
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3789000e+00 -1.4468000e+00 -5.8369000e-02 /
CHEB / 3.2182000e+00 8.4086000e-01 -6.3952000e-02 /
CHEB / 1.4123000e-01 4.6794000e-01 -9.1024000e-03 /
CHEB / -1.9388000e-01 1.6187000e-01 4.0331000e-02 /
CHEB / -1.2356000e-01 -2.7057000e-03 4.9826000e-02 /

tSPC(110)+H(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -80.4612996570353
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2195000e+01 -6.2351000e-01 -2.1429000e-01 /
CHEB / 3.8244000e-01 6.3449000e-01 1.7313000e-01 /
CHEB / -5.4243000e-02 7.1665000e-02 6.7206000e-02 /
CHEB / -2.6008000e-02 -6.2285000e-02 -8.1527000e-03 /
CHEB / 1.2924000e-03 -3.3770000e-02 -1.9667000e-02 /

C4H6Oi-12+H(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -32.59231356126859
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2297000e+01 -2.4123000e-03 -2.5235000e-04 /
CHEB / 8.3911000e-01 -1.8108000e-03 2.7499000e-04 /
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CHEB / -3.2698000e-03 2.6635000e-04 -6.9827000e-04 /
CHEB / 3.0652000e-02 1.9105000e-03 -6.4705000e-04 /
CHEB / 9.1158000e-03 1.7192000e-03 -1.6387000e-05 /

CH3+C3H4O-enone(+m)=C3H7-2+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -25.180245342212093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2497000e+00 -6.0351000e-04 -4.1988000e-04 /
CHEB / 3.0670000e+00 7.1915000e-04 5.0029000e-04 /
CHEB / -1.4713000e-02 -6.2072000e-05 -4.3120000e-05 /
CHEB / 1.5781000e-02 -8.0861000e-05 -5.6269000e-05 /
CHEB / -1.9681000e-03 -1.2221000e-05 -8.5185000e-06 /

HCC[CH3]2+O(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -124.66717134595916
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0050000e+01 1.8231000e+00 -1.0740000e-01 /
CHEB / -9.1438000e-01 2.0839000e-01 1.2250000e-01 /
CHEB / -4.3299000e-01 -1.4905000e-02 -3.7264000e-03 /
CHEB / -9.8535000e-02 -2.3265000e-02 -1.4927000e-02 /
CHEB / -1.5390000e-02 -1.7941000e-03 -2.2445000e-03 /

HCC[CH3]2+O(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Cd_pri_rad     Oa        deltaHrxn(T=298K) = -
124.86710093297168 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0679000e+01 1.8433000e+00 -9.3663000e-02 /
CHEB / -1.3027000e+00 1.8788000e-01 1.0857000e-01 /
CHEB / -3.7388000e-01 -1.5534000e-02 -4.1664000e-03 /
CHEB / -2.1418000e-02 -2.0805000e-02 -1.3276000e-02 /
CHEB / 2.5569000e-02 -1.0642000e-03 -1.7422000e-03 /

HCC[CH3]2+O(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -117.0377615073206
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4595000e+00 1.8436000e+00 -9.3552000e-02 /
CHEB / 1.7185000e-01 1.8809000e-01 1.0878000e-01 /
CHEB / -4.0168000e-02 -1.6014000e-02 -4.4641000e-03 /
CHEB / 7.2911000e-02 -2.0968000e-02 -1.3420000e-02 /
CHEB / 5.8053000e-02 -1.0557000e-03 -1.7439000e-03 /

HCC[CH3]2+O(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -129.1365248468021
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6256000e+00 1.8441000e+00 -9.3165000e-02 /
CHEB / -2.9436000e-01 1.8791000e-01 1.0867000e-01 /
CHEB / -1.1506000e-01 -1.6116000e-02 -4.5260000e-03 /
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CHEB / 8.5460000e-02 -2.0927000e-02 -1.3397000e-02 /
CHEB / 1.0713000e-01 -1.0224000e-03 -1.7232000e-03 /

HCC[CH3]2+O(+m)=iC4H7OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -116.99787745375507
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8226000e+00 1.7199000e+00 -1.7350000e-01 /
CHEB / -4.7250000e-01 3.0678000e-01 1.8428000e-01 /
CHEB / -4.5710000e-01 1.7517000e-03 7.6442000e-03 /
CHEB / -1.5618000e-01 -3.5940000e-02 -2.2444000e-02 /
CHEB / -3.4653000e-02 -8.9040000e-03 -6.9814000e-03 /

HCC[CH3]2+O(+m)=C3H3OH+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -75.4425001968502
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2665000e+01 -1.7346000e-01 -1.0535000e-01 /
CHEB / -3.6525000e-01 2.0829000e-01 1.2271000e-01 /
CHEB / -2.7035000e-01 -1.6918000e-02 -4.9835000e-03 /
CHEB / -1.3636000e-01 -2.3545000e-02 -1.5240000e-02 /
CHEB / -6.0773000e-02 -1.5723000e-03 -2.1205000e-03 /

HCC[CH3]2+O(+m)=C4H6Oi-13+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -93.18089039035206
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7933000e+00 -1.5540000e-01 -9.2905000e-02 /
CHEB / -1.9078000e+00 1.8795000e-01 1.0876000e-01 /
CHEB / -5.9193000e-01 -1.6405000e-02 -4.6998000e-03 /
CHEB / -2.0901000e-01 -2.0985000e-02 -1.3462000e-02 /
CHEB / -8.0388000e-02 -1.0030000e-03 -1.7149000e-03 /

tSPC(110)+H(+m)=HCC[CH3]2+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 39.77629111237137
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.2920000e+00 -1.5062000e-01 -9.0200000e-02 /
CHEB / 1.3617000e+01 1.8692000e-01 1.0865000e-01 /
CHEB / 3.7227000e-01 -2.0030000e-02 -6.9892000e-03 /
CHEB / 2.0526000e-01 -2.1305000e-02 -1.3927000e-02 /
CHEB / 9.0749000e-02 -3.6426000e-04 -1.3126000e-03 /

HCC[CH3]2+O(+m)=C4H6Oi-12+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -87.64527720813808
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6621000e+00 -1.5458000e-01 -9.2408000e-02 /
CHEB / -2.1037000e+00 1.8776000e-01 1.0869000e-01 /
CHEB / -5.9971000e-01 -1.6914000e-02 -5.0224000e-03 /
CHEB / -1.9994000e-01 -2.1044000e-02 -1.3530000e-02 /
CHEB / -7.4688000e-02 -9.3131000e-04 -1.6718000e-03 /
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HCC[CH3]2+O(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -99.78964876216955
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1789000e+01 -1.5522000e-01 -9.2835000e-02 /
CHEB / 3.0295000e-01 1.8801000e-01 1.0885000e-01 /
CHEB / -8.5450000e-02 -1.6799000e-02 -4.9516000e-03 /
CHEB / -5.9546000e-02 -2.1099000e-02 -1.3562000e-02 /
CHEB / -2.8093000e-02 -9.7337000e-04 -1.6990000e-03 /

HCC[CH3]2+O(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -100.34988804152113
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1642000e+01 -1.5519000e-01 -9.2817000e-02 /
CHEB / 7.3365000e-01 1.8801000e-01 1.0885000e-01 /
CHEB / 2.9856000e-02 -1.6820000e-02 -4.9651000e-03 /
CHEB / -1.8640000e-02 -2.1102000e-02 -1.3565000e-02 /
CHEB / -1.1921000e-02 -9.7074000e-04 -1.6975000e-03 /

HCC[CH3]2+O(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -117.5879033857879
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3423000e+00 -1.5111000e-01 -9.0470000e-02 /
CHEB / 2.4125000e+00 1.8695000e-01 1.0860000e-01 /
CHEB / 6.8779000e-01 -1.9730000e-02 -6.8044000e-03 /
CHEB / 2.4495000e-01 -2.1329000e-02 -1.3913000e-02 /
CHEB / 8.5752000e-02 -4.4190000e-04 -1.3641000e-03 /

HCC[CH3]2+O(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -95.05734542719456
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0156000e+01 -1.5383000e-01 -9.1977000e-02 /
CHEB / 2.8426000e-01 1.8770000e-01 1.0873000e-01 /
CHEB / 8.6231000e-02 -1.7482000e-02 -5.3779000e-03 /
CHEB / 5.5306000e-02 -2.1151000e-02 -1.3639000e-02 /
CHEB / 2.7709000e-02 -8.6739000e-04 -1.6359000e-03 /

HCC[CH3]2+O(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -120.23759076940667
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1280000e+01 -1.5532000e-01 -9.2848000e-02 /
CHEB / 2.8181000e-01 1.8788000e-01 1.0871000e-01 /
CHEB / -1.9154000e-02 -1.6462000e-02 -4.7404000e-03 /
CHEB / -8.0389000e-03 -2.0991000e-02 -1.3463000e-02 /
CHEB / -1.4901000e-03 -9.9100000e-04 -1.7070000e-03 /
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aC3H4+CH2OH(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -52.954651543336844
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4536000e+00 -2.5040000e-01 -2.2545000e-01 /
CHEB / 3.0863000e+00 1.6684000e+00 -1.2054000e-01 /
CHEB / -5.1904000e-01 5.9983000e-01 1.5721000e-01 /
CHEB / -3.3371000e-01 2.8048000e-03 1.3377000e-01 /
CHEB / -1.4896000e-01 -1.1861000e-01 2.2495000e-02 /

aC3H4+CH2OH(+m)=iC4H7OJ(30)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -53.15458113034937
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4491000e+00 -6.8935000e-01 -4.1411000e-01 /
CHEB / 2.9877000e+00 2.1791000e+00 7.4532000e-02 /
CHEB / -5.9286000e-01 5.8225000e-01 1.8212000e-01 /
CHEB / -3.7005000e-01 -6.2836000e-02 1.0289000e-01 /
CHEB / -1.6530000e-01 -1.3346000e-01 7.2917000e-03 /

aC3H4+CH2OH(+m)=iC4H7OJ(48)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -45.32524170469828
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2883000e+00 -6.2642000e-01 -4.1357000e-01 /
CHEB / 4.8836000e+00 2.2389000e+00 1.0530000e-01 /
CHEB / -1.3238000e-01 5.4332000e-01 1.9267000e-01 /
CHEB / -2.3778000e-01 -1.0248000e-01 9.4823000e-02 /
CHEB / -1.1286000e-01 -1.4676000e-01 -4.4389000e-03 /

aC3H4+CH2OH(+m)=iC4H7OJ(51)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -57.42400504417978
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.6594000e-01 -6.1027000e-01 -4.0301000e-01 /
CHEB / 4.3579000e+00 2.2364000e+00 1.0052000e-01 /
CHEB / -2.1687000e-01 5.4784000e-01 1.9520000e-01 /
CHEB / -2.3038000e-01 -1.0339000e-01 9.6082000e-02 /
CHEB / -6.9189000e-02 -1.5012000e-01 -5.4189000e-03 /

aC3H4+CH2OH(+m)=iC4H7OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ca_Cd/H2     C_rad/H2/O          deltaHrxn(T=298K)
= -45.28535765113275 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9508000e+00 7.6014000e-01 -1.4350000e-01 /
CHEB / 1.9246000e+00 9.3861000e-01 -3.9541000e-02 /
CHEB / -5.9512000e-01 3.2073000e-01 8.8329000e-02 /
CHEB / -2.1602000e-01 8.2088000e-03 6.8982000e-02 /
CHEB / -5.8460000e-02 -6.0145000e-02 1.4935000e-02 /
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```
aC3H4+CH2OH(+m)=C3H3OH+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -3.729980394227887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7574000e+00 -2.0313000e+00 -2.1725000e-01 /
CHEB / 5.1603000e+00 1.8059000e+00 -4.5073000e-02 /
CHEB / 2.7633000e-02 4.6858000e-01 2.0632000e-01 /
CHEB / -2.9497000e-01 -1.2470000e-01 1.0222000e-01 /
CHEB / -1.6620000e-01 -1.5619000e-01 -2.6033000e-02 /

C4H6Oi-13+H(+m)=aC3H4+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 21.468370587729737
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0699000e+00 -2.5584000e+00 -3.8418000e-01 /
CHEB / 1.0676000e+01 2.2331000e+00 9.3957000e-02 /
CHEB / -3.6529000e-01 5.3858000e-01 2.0378000e-01 /
CHEB / -3.7284000e-01 -1.1897000e-01 9.3639000e-02 /
CHEB / -1.7954000e-01 -1.5722000e-01 -1.1236000e-02 /

tSPC(110)+H(+m)=aC3H4+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -31.936228690250946
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1470000e+01 -1.2962000e+00 -4.6416000e-01 /
CHEB / 7.8488000e-01 1.3394000e+00 3.9422000e-01 /
CHEB / -6.8542000e-02 1.4091000e-01 1.3388000e-01 /
CHEB / -1.5359000e-01 -1.4774000e-01 -3.0895000e-02 /
CHEB / -8.3134000e-02 -7.9560000e-02 -4.6372000e-02 /

C4H6Oi-12+H(+m)=aC3H4+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 15.932757405515764
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4996000e+00 -2.5190000e+00 -3.9293000e-01 /
CHEB / 9.1425000e+00 2.2823000e+00 1.2733000e-01 /
CHEB / -2.2217000e-01 4.9175000e-01 2.0666000e-01 /
CHEB / -3.4395000e-01 -1.5022000e-01 8.3988000e-02 /
CHEB / -1.7847000e-01 -1.6199000e-01 -2.1123000e-02 /

aC3H4+CH2OH(+m)=C3H6+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -28.077128959547224
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3966000e+00 -2.5364000e+00 -4.0161000e-01 /
CHEB / 5.4630000e+00 2.2889000e+00 1.3272000e-01 /
CHEB / -5.2287000e-02 4.9251000e-01 2.0423000e-01 /
CHEB / -3.3898000e-01 -1.4823000e-01 8.3701000e-02 /
CHEB / -1.8564000e-01 -1.6022000e-01 -1.9706000e-02 /
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aC3H4+CH2OH(+m)=C3H4O+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -28.63736823889881
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2151000e+00 -2.5337000e+00 -4.0134000e-01 /
CHEB / 5.9093000e+00 2.2899000e+00 1.3345000e-01 /
CHEB / 6.6857000e-02 4.9065000e-01 2.0451000e-01 /
CHEB / -2.9727000e-01 -1.4955000e-01 8.3301000e-02 /
CHEB / -1.6915000e-01 -1.6043000e-01 -2.0164000e-02 /

aC3H4+CH2OH(+m)=C3H7-1+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -45.875383583165586
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1470000e+00 -1.6257000e+00 -4.8207000e-01 /
CHEB / 1.2641000e+01 1.6892000e+00 3.8190000e-01 /
CHEB / 5.7121000e-01 1.6584000e-01 1.6236000e-01 /
CHEB / -1.1954000e-02 -1.8324000e-01 -1.9924000e-02 /
CHEB / -5.4163000e-02 -9.8343000e-02 -5.3295000e-02 /

aC3H4+CH2OH(+m)=CH3+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -23.34482562457226
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8566000e+00 -2.4621000e+00 -3.8623000e-01 /
CHEB / 5.7320000e+00 2.3082000e+00 1.4448000e-01 /
CHEB / 1.9818000e-01 4.5204000e-01 2.1170000e-01 /
CHEB / -2.1122000e-01 -1.8126000e-01 7.4022000e-02 /
CHEB / -1.2833000e-01 -1.6780000e-01 -3.1612000e-02 /

aC3H4+CH2OH(+m)=C3H7-2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -48.525070966784355
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4891000e+00 -2.5764000e+00 -3.9771000e-01 /
CHEB / 5.0816000e+00 2.2597000e+00 1.1210000e-01 /
CHEB / -7.5370000e-02 5.3139000e-01 2.0021000e-01 /
CHEB / -3.1137000e-01 -1.2172000e-01 9.2127000e-02 /
CHEB / -1.7222000e-01 -1.5712000e-01 -1.1435000e-02 /

HCC[CH3]2+O(+m)=aC3H4+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -71.71251980262231
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1001000e+01 -2.7260000e-01 -1.6884000e-01 /
CHEB / 2.1803000e-01 3.0718000e-01 1.8498000e-01 /
CHEB / -2.1263000e-01 -2.6527000e-03 4.9227000e-03 /
CHEB / -1.6537000e-01 -3.6797000e-02 -2.3212000e-02 /
CHEB / -9.2331000e-02 -8.3533000e-03 -6.6968000e-03 /
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iC4H7OJ(15)(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 23.52771939648573
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1361000e+01 -1.3200000e-01 3.4992000e-02 /
CHEB / 1.8379000e+01 1.5163000e+00 -2.3141000e-01 /
CHEB / -6.0235000e-01 5.2107000e-01 -4.6739000e-02 /
CHEB / -3.6780000e-01 1.2168000e-01 1.4000000e-01 /
CHEB / -1.2510000e-01 -5.2988000e-02 8.0885000e-02 /

iC4H7OJ(30)(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 23.727648983498256
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1580000e+01 -6.6854000e-01 -1.4826000e-01 /
CHEB / 1.8598000e+01 2.1196000e+00 -6.9544000e-02 /
CHEB / -6.1395000e-01 5.2289000e-01 1.0667000e-02 /
CHEB / -3.9779000e-01 5.1321000e-02 1.1342000e-01 /
CHEB / -1.4997000e-01 -8.0355000e-02 5.7526000e-02 /

iC4H7OJ(48)(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 15.898309557847167
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3935000e+01 -5.0912000e-01 -1.4492000e-01 /
CHEB / 1.8200000e+01 2.1211000e+00 -6.8571000e-02 /
CHEB / -5.1736000e-02 4.7428000e-01 4.7459000e-02 /
CHEB / -2.0972000e-01 -3.1600000e-03 1.1576000e-01 /
CHEB / -6.4452000e-02 -1.1011000e-01 4.4192000e-02 /

iC4H7OJ(51)(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 27.99707289732866
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0268000e+01 -5.0381000e-01 -1.3016000e-01 /
CHEB / 2.1756000e+01 2.1288000e+00 -7.5898000e-02 /
CHEB / -1.1072000e-01 4.8121000e-01 4.5148000e-02 /
CHEB / -1.8389000e-01 -2.2799000e-03 1.1909000e-01 /
CHEB / -7.1482000e-03 -1.1436000e-01 4.4654000e-02 /

iC4H7OJ(17)(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 15.85842550428163
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.1861000e+00 5.9383000e-01 -1.0136000e-01 /
CHEB / 1.4220000e+01 8.9953000e-01 -9.2097000e-02 /
CHEB / -6.2356000e-01 4.1676000e-01 3.7692000e-02 /
CHEB / -2.7244000e-01 7.8214000e-02 7.2715000e-02 /
CHEB / -8.7548000e-02 -4.4548000e-02 3.9873000e-02 /
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C3H3OH+CH3(+m)=C4H7OJ(79)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -25.696951752623228
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7592000e+00 -1.6421000e+00 5.9370000e-02 /
CHEB / 5.1490000e+00 1.4126000e+00 -2.6439000e-01 /
CHEB / 2.5673000e-01 4.1093000e-01 9.6396000e-02 /
CHEB / -1.2215000e-01 -4.4848000e-02 1.3581000e-01 /
CHEB / -5.8302000e-02 -1.2818000e-01 1.7867000e-02 /

C4H6Oi-13+H(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -7.958561559121382
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9714000e+00 -2.4224000e+00 -1.0589000e-01 /
CHEB / 8.9776000e+00 2.1016000e+00 -9.7359000e-02 /
CHEB / -1.1191000e-01 4.7293000e-01 6.1107000e-02 /
CHEB / -2.5671000e-01 -2.1674000e-02 1.2114000e-01 /
CHEB / -9.5669000e-02 -1.2688000e-01 3.8606000e-02 /

C4H6Oi-12+H(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -13.494174741335353
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1712000e+00 -2.3159000e+00 -1.1706000e-01 /
CHEB / 7.6560000e+00 2.0927000e+00 -7.9396000e-02 /
CHEB / 5.4207000e-02 4.2492000e-01 8.4462000e-02 /
CHEB / -2.1368000e-01 -6.4396000e-02 1.1506000e-01 /
CHEB / -8.9724000e-02 -1.3872000e-01 2.4939000e-02 /

C3H6+HCO(+m)=C4H7OJ(79)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -1.3498031873038876
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5825000e+00 -2.3442000e+00 -1.3092000e-01 /
CHEB / 1.3725000e+01 2.1126000e+00 -6.5847000e-02 /
CHEB / 3.1210000e-01 4.2343000e-01 8.0261000e-02 /
CHEB / -1.7623000e-01 -6.2831000e-02 1.1336000e-01 /
CHEB / -7.8754000e-02 -1.3582000e-01 2.6562000e-02 /

C3H4O+CH3(+m)=C4H7OJ(79)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -0.78956390795231
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3762000e+00 -2.3389000e+00 -1.3064000e-01 /
CHEB / 1.4099000e+01 2.1114000e+00 -6.5817000e-02 /
CHEB / 3.3235000e-01 4.2162000e-01 8.1264000e-02 /
CHEB / -1.4765000e-01 -6.4593000e-02 1.1314000e-01 /
CHEB / -6.1317000e-02 -1.3630000e-01 2.5962000e-02 /
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C3H7-1+CO(+m)=C4H7OJ(79)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 16.448451436314468
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5722000e+01 -1.1704000e+00 -2.7743000e-01 /
CHEB / 2.8605000e+01 1.2167000e+00 1.9544000e-01 /
CHEB / 8.2636000e-01 1.2477000e-01 1.1775000e-01 /
CHEB / 1.7534000e-01 -1.2920000e-01 -3.1939000e-04 /
CHEB / 4.7653000e-02 -7.0663000e-02 -3.4646000e-02 /

CH3+C3H4O-enone(+m)=C4H7OJ(79)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -6.082106522278856
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7713000e+00 -2.2309000e+00 -1.1195000e-01 /
CHEB / 1.2376000e+01 2.0949000e+00 -7.2331000e-02 /
CHEB / 5.7316000e-01 3.8500000e-01 9.9842000e-02 /
CHEB / -3.0294000e-02 -1.0346000e-01 1.0962000e-01 /
CHEB / -2.1031000e-02 -1.5029000e-01 1.1893000e-02 /

C3H7-2+CO(+m)=C4H7OJ(79)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = 19.098138819933236
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4407000e+01 -2.4447000e+00 -1.2386000e-01 /
CHEB / 2.0180000e+01 2.1353000e+00 -7.4155000e-02 /
CHEB / 3.0411000e-01 4.6387000e-01 5.7538000e-02 /
CHEB / -1.5182000e-01 -2.5642000e-02 1.1920000e-01 /
CHEB / -6.9259000e-02 -1.2721000e-01 3.8206000e-02 /

HCC[CH3]2+O(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -101.13945194947343
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0157000e+01 -1.8081000e-01 -1.0970000e-01 /
CHEB / 7.1793000e-01 2.1454000e-01 1.2623000e-01 /
CHEB / 1.8797000e-02 -1.4377000e-02 -3.3391000e-03 /
CHEB / -3.6213000e-02 -2.4309000e-02 -1.5578000e-02 /
CHEB / -2.1882000e-02 -2.4229000e-03 -2.6553000e-03 /

aC3H4+CH2OH(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -29.426932146851115
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4534000e+00 -1.1515000e+00 -1.3952000e-01 /
CHEB / 4.5078000e+00 1.0030000e+00 -8.3903000e-03 /
CHEB / 2.1348000e-01 2.7037000e-01 1.0994000e-01 /
CHEB / -8.1115000e-02 -5.0522000e-02 5.8031000e-02 /
CHEB / -7.4965000e-02 -8.3144000e-02 -6.4466000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
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```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     pC3H3             81.58 59.57 13.76 16.14 18.14 19.8  22.39 24.34
      27.47 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     pC3H3+H=aC3H4           5.3600000e+14      0.00000
9.8000000e+02

pC3H3+H(+m)=aC3H4(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (aC3H4) High-P Limit: R_Recombination exact:  Cd_pri_rad     H_rad
      deltaHrxn(T=298K) = -83.8508609923952 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4424000e+01 1.0526000e-02 -6.2604000e-03 /
CHEB / 3.2269000e-01 2.0269000e-02 -1.2026000e-02 /
CHEB / 2.0592000e-02 1.8158000e-02 -1.0703000e-02 /
CHEB / 6.1942000e-02 1.5167000e-02 -8.8500000e-03 /
CHEB / 3.6432000e-02 1.1808000e-02 -6.8014000e-03 /

!PDepNetwork pC3H4
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     pC3H4             46.16 58.99 14.37 17.14 19.55 21.6  24.93 27.49
      31.65
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H               137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     pC3H3             86.21 60.63 14.9  17.21 19.0  20.43 22.68 24.42
      27.32
!Here are the path reactions and their high-P limit kinetics:
!     C2H+CH3=pC3H4           1.4157154e+13      -0.15000
2.9166667e+02
!     pC3H3+H=pC3H4           6.400e+13    0.10        -30.00

C2H+CH3(+m)=pC3H4(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (pC3H4) High-P Limit: R_Recombination estimate: (Average:) Ct_rad
C_methyl          deltaHrxn(T=298K) = -126.21645447092729 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6960000e+00 6.6867000e+00 -8.4272000e-02 /
CHEB / -3.8726000e+00 1.5556000e-01 6.7573000e-01 /
CHEB / -1.6338000e+00 -2.0674000e-01 8.5090000e-02 /
CHEB / -6.8314000e-01 -1.2087000e-01 -6.1123000e-03 /
CHEB / -2.9325000e-01 -5.3269000e-02 -7.9927000e-03 /
```

```
pC3H3+H(+m)=pC3H4(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (pC3H4) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -92.13990534188414 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3395000e+01 4.8758000e-01 -6.6895000e-02 /
CHEB / -1.1811000e+00 7.4798000e-01 -5.3366000e-02 /
CHEB / -8.4615000e-01 3.8757000e-01 2.3685000e-02 /
CHEB / -4.7603000e-01 1.2777000e-01 3.8696000e-02 /
CHEB / -2.4833000e-01 1.0555000e-02 1.9796000e-02 /

C2H+CH3(+m)=pC3H3+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (pC3H4)  deltaHrxn(T=298K) = -34.07654912904314 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2804000e+01 -5.8437000e-02 -4.5593000e-02 /
CHEB / -5.2182000e-02 8.0868000e-02 6.2269000e-02 /
CHEB / -1.2400000e-02 -1.9465000e-02 -1.3523000e-02 /
CHEB / 4.5162000e-02 -5.7692000e-03 -5.4498000e-03 /
CHEB / 2.7676000e-02 1.5815000e-03 1.1844000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H6-12           38.85 69.81 19.35 23.63 27.42 30.79 36.04 39.99
      46.09 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     sSPC(46)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04
!     sSPC(46)=HO2+C4H6-13    4.3669559e+09      1.31333
2.9866667e+04
!     CH3CH[o]C2H3+O=sSPC(46) 1.0000000e+13      0.00000
0.0000000e+00

CH3CH[o]C2H3+O(+m)=sSPC(46)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #113 (sSPC(46)) High-P Limit: Oa_R_Recombination estimate:
```

```
(Average:) O_rad/NonDe     Oa       deltaHrxn(T=298K) = -
59.20385145591645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7963000e+00 1.9833000e+00 -1.1491000e-02 /
CHEB / -9.8344000e-01 1.6493000e-02 1.1315000e-02 /
CHEB / -4.1922000e-01 2.8592000e-03 1.9839000e-03 /
CHEB / -7.8918000e-02 -2.3418000e-03 -1.5960000e-03 /
CHEB / 2.9131000e-02 -1.2731000e-03 -8.8087000e-04 /

CH3CH[o]C2H3+O(+m)=HO2+C4H6-12(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #113 (sSPC(46))   deltaHrxn(T=298K) = -32.97664936605182
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0241000e+01 -1.5665000e-02 -1.0775000e-02 /
CHEB / 1.1852000e+00 1.6340000e-02 1.1216000e-02 /
CHEB / 2.8479000e-01 1.9728000e-03 1.3771000e-03 /
CHEB / 4.1529000e-02 -2.4689000e-03 -1.6871000e-03 /
CHEB / -1.9730000e-02 -1.0254000e-03 -7.1274000e-04 /

CH3CH[o]C2H3+O(+m)=HO2+C4H6-13(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #113 (sSPC(46))   deltaHrxn(T=298K) = -45.745257650558564
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1070000e+01 -1.5665000e-02 -1.0775000e-02 /
CHEB / 1.5003000e+00 1.6340000e-02 1.1216000e-02 /
CHEB / 3.6758000e-01 1.9728000e-03 1.3771000e-03 /
CHEB / 7.0535000e-02 -2.4689000e-03 -1.6871000e-03 /
CHEB / -8.3126000e-03 -1.0254000e-03 -7.1274000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H6-12           38.85 69.81 19.35 23.63 27.42 30.79 36.04 39.99
      46.09 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
!     nSPC(102)+pC3H5=sSPC(56)      1.4157154e+13      -0.15000
2.9166667e+02
!     sSPC(56)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04

nSPC(102)+pC3H5(+m)=HO2+C4H6-12(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #163 (sSPC(56))   deltaHrxn(T=298K) = -75.57229002361845
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0622000e+01 -7.9187000e-03 -5.4808000e-03 /
CHEB / 9.0752000e-01 8.3773000e-03 5.7897000e-03 /
CHEB / 2.0662000e-01 9.4297000e-05 7.3198000e-05 /
CHEB / 6.6289000e-02 -1.0850000e-03 -7.5063000e-04 /
CHEB / 7.6187000e-03 -3.7791000e-04 -2.6377000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2C[OH]CH2 -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26 40.88
      null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     pC3H4             44.28 59.28 14.6  17.31 19.7  21.75 25.09 27.65
      32.78 null
!     CH3C[OH]cH  20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23 39.84
      null
!Here are the path reactions and their high-P limit kinetics:

aC3H4+HOC[CH2][CH3]2(+m)=CH2C[OH]CH2+iC4H8(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H13OJ(332)) deltaHrxn(T=298K)
= -27.127250465196365 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4979000e+00 -1.2939000e+00 -8.7932000e-02 /
CHEB / 1.0959000e+01 1.0261000e+00 -3.0516000e-02 /
CHEB / 4.9705000e-01 4.4710000e-01 8.9715000e-02 /
CHEB / -3.5388000e-01 5.1420000e-02 8.3465000e-02 /
CHEB / -2.9031000e-01 -1.0347000e-01 1.5249000e-02 /
```

```
aC3H4+HOC[CH2][CH3]2(+m)=pC3H4+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H13OJ(332)) deltaHrxn(T=298K)
= -2.4398051299241956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1701000e+00 -1.4808000e+00 -1.9484000e-01 /
CHEB / 1.0720000e+01 1.3189000e+00 1.2065000e-01 /
CHEB / 3.8905000e-01 3.3034000e-01 4.7598000e-02 /
CHEB / -4.5247000e-01 4.4516000e-02 7.3219000e-02 /
CHEB / -3.2642000e-01 -8.7017000e-02 2.4060000e-02 /

pC3H4+HOC[CH2][CH3]2(+m)=CH2C[OH]CH2+iC4H8(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H13OJ(332)) deltaHrxn(T=298K)
= -24.68744533527217 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.6107000e+00 -1.4396000e+00 -1.9572000e-01 /
CHEB / 1.4082000e+01 1.2857000e+00 1.1615000e-01 /
CHEB / 7.5909000e-01 3.1988000e-01 5.3779000e-02 /
CHEB / -3.1702000e-01 3.6782000e-02 7.4133000e-02 /
CHEB / -2.7292000e-01 -8.7247000e-02 2.0439000e-02 /

aC3H4+HOC[CH2][CH3]2(+m)=CH3C[OH]cH+iC4H8(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H13OJ(332)) deltaHrxn(T=298K)
= -4.1296615557761065 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2359000e+01 -1.2687000e+00 -2.3545000e-01 /
CHEB / 1.8455000e+01 1.1869000e+00 1.5760000e-01 /
CHEB / 7.4616000e-01 2.5934000e-01 7.7698000e-02 /
CHEB / -1.8997000e-01 -1.5950000e-02 5.7352000e-02 /
CHEB / -1.9765000e-01 -9.4563000e-02 -1.4390000e-04 /

CH3C[OH]cH+iC4H8(+m)=pC3H4+HOC[CH2][CH3]2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C7H13OJ(332)) deltaHrxn(T=298K)
= 1.6898564258519109 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9605000e+00 -1.1342000e-01 -7.0788000e-02 /
CHEB / 1.6087000e+01 1.6853000e-01 1.0340000e-01 /
CHEB / 3.1752000e-01 -5.9286000e-02 -3.2916000e-02 /
CHEB / 8.0313000e-02 -2.7175000e-03 -4.9641000e-03 /
CHEB / 8.2894000e-03 7.7209000e-03 5.6082000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OC[CH3]3    -23.14      76.55 26.22 32.91 38.66 43.41 50.9  56.36
      64.83 null
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tC4H9       11.9  74.29 22.33 27.04 31.82 36.27 43.62 49.34 58.52
      null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH2C[OH]CH2 -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26 40.88
      null
!     pC3H4             44.28 59.28 14.6  17.31 19.7  21.75 25.09 27.65
      32.78 null
!     CH3C[OH]cH  20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23 39.84
      null
!Here are the path reactions and their high-P limit kinetics:

OC[CH3]3+aC3H4(+m)=iC4H8+CH2C[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (C7H13OJ(358)) deltaHrxn(T=298K) = -
30.08698852391195 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0540000e+00 -1.0362000e+00 -1.8866000e-01 /
CHEB / 9.6213000e+00 8.8166000e-01 7.6667000e-02 /
CHEB / 5.3588000e-01 3.0048000e-01 1.1646000e-01 /
CHEB / -1.8711000e-01 3.7261000e-03 5.6059000e-02 /
CHEB / -2.2684000e-01 -7.6154000e-02 -8.7280000e-03 /

OC[CH3]3+aC3H4(+m)=pC3H4+OC[CH3]3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (C7H13OJ(358)) deltaHrxn(T=298K) = -
2.4398051299241956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6212000e+00 -1.1785000e+00 -2.2550000e-01 /
CHEB / 8.1757000e+00 1.0864000e+00 1.3556000e-01 /
CHEB / 6.2972000e-01 2.3215000e-01 8.7731000e-02 /
CHEB / -2.3414000e-01 6.4822000e-03 6.0915000e-02 /
CHEB / -2.5301000e-01 -7.1369000e-02 -4.5474000e-03 /

pC3H4+OC[CH3]3(+m)=iC4H8+CH2C[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (C7H13OJ(358)) deltaHrxn(T=298K) = -
27.647183393987753 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1733000e+00 -1.0652000e+00 -2.3309000e-01 /
CHEB / 1.2511000e+01 9.8582000e-01 1.4810000e-01 /
CHEB / 9.0912000e-01 2.1539000e-01 9.1054000e-02 /
CHEB / -1.1605000e-01 -9.9609000e-03 4.9037000e-02 /
CHEB / -2.0298000e-01 -7.1636000e-02 -1.1639000e-02 /

OC[CH3]3+aC3H4(+m)=CH3C[OH]cH+iC4H8(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (C7H13OJ(358)) deltaHrxn(T=298K) = -
7.08939961449169 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0015000e+01 -7.5232000e-01 -2.6752000e-01 /
CHEB / 1.7331000e+01 7.2396000e-01 2.2332000e-01 /
CHEB / 6.3896000e-01 1.5755000e-01 8.1086000e-02 /
CHEB / -4.0081000e-02 -4.5305000e-02 1.0515000e-02 /
CHEB / -1.3274000e-01 -6.6465000e-02 -2.4669000e-02 /
```

```
CH3C[OH]cH+iC4H8(+m)=iC4H8+CH2C[OH]CH2(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #13 (C7H13OJ(358))
      deltaHrxn(T=298K) = -22.99758890942026 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8000000e+01 -7.7220000e-01 -2.5897000e-01 /
CHEB / 2.1970000e+01 7.6529000e-01 2.1872000e-01 /
CHEB / 1.2972000e+00 1.3628000e-01 7.6390000e-02 /
CHEB / 1.5535000e-01 -5.7353000e-02 6.1730000e-03 /
CHEB / -6.1219000e-02 -6.3931000e-02 -2.5293000e-02 /

pC3H4+OC[CH3]3(+m)=CH3C[OH]cH+iC4H8(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #13 (C7H13OJ(358)) deltaHrxn(T=298K) = -
4.649594484567494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2461000e+00 -2.0963000e-02 -1.4832000e-02 /
CHEB / 1.5575000e+01 3.0732000e-02 2.1803000e-02 /
CHEB / 1.7344000e-01 -1.0472000e-02 -7.5399000e-03 /
CHEB / 5.7351000e-02 -2.4531000e-04 -7.2174000e-05 /
CHEB / -7.6032000e-03 1.0464000e-03 7.1253000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H5O2J(54) 21.86 78.59 23.19 28.36 32.19 35.33 39.81 42.82 47.49
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

HO2+C4H7-24(+m)=CH3CH[o]C2H3+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(353))  deltaHrxn(T=298K) = -11.27913697724784
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2217000e+01 -5.6002000e-01 -1.8523000e-01 /
CHEB / 4.7575000e-01 6.6015000e-01 1.9023000e-01 /
CHEB / -5.6943000e-02 -4.0882000e-03 3.7114000e-02 /
```

```
CHEB / -8.3908000e-02 -9.3325000e-02 -2.8959000e-02 /
CHEB / -2.8570000e-02 -2.3353000e-02 -2.0321000e-02 /

sSPC(46)+H(+m)=CH3CH[o]C2H3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(353))  deltaHrxn(T=298K) = -40.01574354563737
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3033000e+01 -1.4299000e-03 -1.2197000e-03 /
CHEB / -2.6354000e-01 1.7111000e-03 1.4593000e-03 /
CHEB / -1.2638000e-03 8.1810000e-05 6.8851000e-05 /
CHEB / 4.5745000e-02 -4.7142000e-04 -4.0025000e-04 /
CHEB / 2.6662000e-02 6.1102000e-06 5.0305000e-06 /

sSPC(46)+H(+m)=HO2+C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(353))  deltaHrxn(T=298K) = -28.736606568389526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0967000e+01 -9.0249000e-03 -6.4614000e-03 /
CHEB / -3.2507000e-02 1.0435000e-02 7.4914000e-03 /
CHEB / 1.5015000e-01 3.3227000e-04 2.1496000e-04 /
CHEB / 8.9591000e-02 -1.8560000e-03 -1.3378000e-03 /
CHEB / 3.3595000e-02 -2.3360000e-04 -1.5660000e-04 /

C3H5O2J(54)+CH3(+m)=CH3CH[o]C2H3+OH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O2(353))   deltaHrxn(T=298K) = -
34.636245908592834 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2918000e+01 -1.5355000e-02 -1.2726000e-02 /
CHEB / -2.6107000e-01 1.9038000e-02 1.5781000e-02 /
CHEB / -6.6757000e-02 -7.0428000e-04 -6.0157000e-04 /
CHEB / 1.8826000e-02 -3.8911000e-03 -3.1953000e-03 /
CHEB / 1.6385000e-02 1.0176000e-04 7.4634000e-05 /

C3H5O2J(54)+CH3(+m)=HO2+C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(353))  deltaHrxn(T=298K) = -23.357108931344996
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0682000e+01 -3.0845000e-02 -2.2022000e-02 /
CHEB / 9.2598000e-02 3.7827000e-02 2.7045000e-02 /
CHEB / 1.1334000e-01 -1.8883000e-03 -1.4096000e-03 /
CHEB / 6.3493000e-02 -6.1792000e-03 -4.3899000e-03 /
CHEB / 2.1377000e-02 -3.6574000e-05 -2.5539000e-05 /

sSPC(46)+H(+m)=C3H5O2J(54)+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(353))  deltaHrxn(T=298K) = -5.37949763704453
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0478000e+00 -1.6881000e-02 -1.1570000e-02 /
CHEB / 2.3000000e+00 2.2034000e-02 1.5072000e-02 /
CHEB / 7.7091000e-01 -3.5384000e-03 -2.3774000e-03 /
CHEB / 2.1925000e-01 -2.2835000e-03 -1.5746000e-03 /
CHEB / 6.1812000e-02 3.4243000e-04 2.2039000e-04 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+H(+m)=HO2+C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H8O2(354))  deltaHrxn(T=298K) = -30.30643339499415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0813000e+01 -6.5573000e-03 -4.7173000e-03 /
CHEB / 2.5418000e-01 7.4535000e-03 5.3796000e-03 /
CHEB / 1.7124000e-01 3.5679000e-04 2.3803000e-04 /
CHEB / 1.0211000e-01 -1.2297000e-03 -8.9326000e-04 /
CHEB / 3.9492000e-02 -2.7229000e-04 -1.8800000e-04 /

CH2OOH+pC3H5(+m)=HO2+C4H7-24(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H8O2(354))  deltaHrxn(T=298K) = -45.44511500812861
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0771000e+01 -8.9041000e-04 -6.2273000e-04 /
CHEB / 2.9148000e-01 8.9344000e-04 6.2519000e-04 /
CHEB / 1.2356000e-01 1.7339000e-04 1.2104000e-04 /
CHEB / 6.7956000e-02 -1.2522000e-04 -8.7896000e-05 /
CHEB / 2.4870000e-02 -6.9581000e-05 -4.8599000e-05 /

sSPC(56)+H(+m)=CH2OOH+pC3H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H8O2(354))  deltaHrxn(T=298K) = 15.138681613134466
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5092000e+00 -3.7667000e-03 -2.6168000e-03 /
CHEB / 6.9785000e+00 4.4952000e-03 3.1222000e-03 /
CHEB / 9.1172000e-01 -1.5163000e-04 -1.0453000e-04 /
CHEB / 2.9876000e-01 -6.3236000e-04 -4.3908000e-04 /
CHEB / 8.2191000e-02 -5.4830000e-05 -3.8438000e-05 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     CH3CH[O]C2H5      -18.47      82.48 26.0  32.47 38.36 43.0  50.56
      56.09 64.77 null
!     C2H5              28.6  59.87 11.73 14.47 17.05 19.34 23.02 25.91
      31.53 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C4H9-2            16.09 80.42 21.84 26.81 31.81 36.38 43.83 49.58
      59.02 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C4H8-1            -0.11 73.61 20.57 26.09 31.04 35.28 41.96 46.97
      54.75 null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[o]C2H3+C4H9-2(+m)=C4H7-24+CH3CH[O]C2H5(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K)
= -14.388650931437411 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6591000e+00 -1.4474000e+00 -2.1834000e-02 /
CHEB / 4.3425000e+00 9.6359000e-01 -2.3685000e-02 /
CHEB / 5.0338000e-01 6.1154000e-01 1.7575000e-02 /
CHEB / -4.6565000e-01 2.1585000e-01 4.2181000e-02 /
CHEB / -3.9717000e-01 -7.1034000e-02 2.8700000e-02 /

C4H7-24+CH3CH[O]C2H5(+m)=C4H6-13+sBuOH(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K)
= -58.754035028470035 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0331000e+00 -1.4776000e+00 -1.0776000e-02 /
CHEB / 5.2474000e+00 9.3117000e-01 -1.2002000e-02 /
CHEB / 6.9187000e-01 6.3677000e-01 8.1041000e-03 /
CHEB / -4.3024000e-01 2.7512000e-01 2.0851000e-02 /
CHEB / -4.5627000e-01 -3.1390000e-02 1.5026000e-02 /
```

```
CH3CH[o]C2H3+C4H9-2(+m)=C4H6-13+sBuOH(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C8H16O(463))   deltaHrxn(T=298K) = -
73.14268595990745 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4583000e+00 -1.4566000e+00 -1.5131000e-02 /
CHEB / 3.8927000e+00 9.5700000e-01 -1.5567000e-02 /
CHEB / 5.6822000e-01 6.2793000e-01 1.4723000e-02 /
CHEB / -3.8843000e-01 2.4216000e-01 3.2259000e-02 /
CHEB / -3.9775000e-01 -5.9866000e-02 2.0506000e-02 /

C4H7-24+CH3CH[O]C2H5(+m)=sC4H8O+C4H8-1(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K)
= -53.76440016874384 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9239000e+00 -1.4745000e+00 -1.2128000e-02 /
CHEB / 5.7007000e+00 9.3447000e-01 -1.3460000e-02 /
CHEB / 7.0443000e-01 6.3388000e-01 9.2350000e-03 /
CHEB / -4.4147000e-01 2.6855000e-01 2.3544000e-02 /
CHEB / -4.4841000e-01 -3.5700000e-02 1.6860000e-02 /

CH3CH[o]C2H3+C4H9-2(+m)=sC4H8O+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C8H16O(463))   deltaHrxn(T=298K) = -
68.15305110018126 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5086000e+00 -1.4546000e+00 -1.7131000e-02 /
CHEB / 4.1729000e+00 9.5789000e-01 -1.8038000e-02 /
CHEB / 6.0679000e-01 6.2295000e-01 1.5472000e-02 /
CHEB / -3.9277000e-01 2.3501000e-01 3.5180000e-02 /
CHEB / -3.9084000e-01 -6.2279000e-02 2.3039000e-02 /

C4H6-13+sBuOH(+m)=sC4H8O+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K) = 4.989634859726192
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6961000e+01 -1.4899000e+00 -8.5983000e-03 /
CHEB / 2.4059000e+01 9.1491000e-01 -1.0242000e-02 /
CHEB / 1.0468000e+00 6.3890000e-01 4.6378000e-03 /
CHEB / -3.3667000e-01 2.9155000e-01 1.4772000e-02 /
CHEB / -4.4021000e-01 -1.4435000e-02 1.1924000e-02 /

C4H7-24+CH3CH[O]C2H5(+m)=sC4H8O+C4H8-2(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K)
= -56.8741402074529 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3259000e+00 -1.4727000e+00 -1.2866000e-02 /
CHEB / 5.9214000e+00 9.3637000e-01 -1.4256000e-02 /
CHEB / 6.9587000e-01 6.3230000e-01 9.8450000e-03 /
CHEB / -4.5016000e-01 2.6488000e-01 2.4998000e-02 /
CHEB / -4.4545000e-01 -3.8142000e-02 1.7848000e-02 /
```

```
CH3CH[o]C2H3+C4H9-2(+m)=sC4H8O+C4H8-2(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C8H16O(463))   deltaHrxn(T=298K) = -
71.26279113889031 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9959000e+00 -1.4533000e+00 -1.8177000e-02 /
CHEB / 4.2982000e+00 9.5874000e-01 -1.9317000e-02 /
CHEB / 6.1531000e-01 6.2041000e-01 1.5890000e-02 /
CHEB / -3.9883000e-01 2.3105000e-01 3.6717000e-02 /
CHEB / -3.8851000e-01 -6.3870000e-02 2.4340000e-02 /

sC4H8O+C4H8-2(+m)=C4H6-13+sBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K) = -1.8798948210171318
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7251000e+01 -1.4873000e+00 -9.0506000e-03 /
CHEB / 2.3983000e+01 9.1851000e-01 -1.0613000e-02 /
CHEB / 1.1010000e+00 6.3866000e-01 5.3470000e-03 /
CHEB / -3.1415000e-01 2.8822000e-01 1.6034000e-02 /
CHEB / -4.2658000e-01 -1.8099000e-02 1.2590000e-02 /

sC4H8O+C4H8-2(+m)=sC4H8O+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C8H16O(463))  deltaHrxn(T=298K) = 3.1097400387090604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7472000e+01 -1.4832000e+00 -1.0096000e-02 /
CHEB / 2.4567000e+01 9.2360000e-01 -1.1612000e-02 /
CHEB / 1.0842000e+00 6.3717000e-01 6.5876000e-03 /
CHEB / -3.2594000e-01 2.8198000e-01 1.8523000e-02 /
CHEB / -4.1859000e-01 -2.3708000e-02 1.4074000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
```

```
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     sSPC(46)+H2O=sSPC(116)  6.5200000e+01      2.92000
5.0700000e+04
!     sSPC(116)=HO2+sC4H8O    8.8110000e+09      1.17000
3.0100000e+04
!     sSPC(116)=HO2+MEKenol   6.4800000e+10      0.57000
2.9900000e+04

sC4H8O+HO2(+m)=sSPC(116)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(370)) deltaHrxn(T=298K) = -19.47809882439146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0972000e+00 1.0606000e+00 -8.8252000e-02 /
CHEB / -3.7900000e+00 1.6130000e+00 -9.4976000e-02 /
CHEB / -5.2684000e+00 5.6167000e-01 2.7843000e-02 /
CHEB / -2.5509000e+00 -2.0264000e-01 4.5230000e-02 /
CHEB / -7.1558000e-01 -3.3009000e-01 -8.6660000e-03 /

MEKenol+HO2(+m)=sSPC(116)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(370)) deltaHrxn(T=298K) = -12.048750909585245
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2321000e+00 7.4867000e-01 -8.9463000e-02 /
CHEB / -1.6127000e+00 1.8863000e+00 -6.8755000e-02 /
CHEB / -5.2303000e+00 4.4639000e-01 4.6265000e-02 /
CHEB / -2.5594000e+00 -2.2893000e-01 2.5842000e-02 /
CHEB / -7.1759000e-01 -3.1406000e-01 -1.4361000e-02 /

sSPC(46)+H2O(+m)=sSPC(116)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(370)) High-P Limit: 1,3_Insertion_ROR exact:
Cd/H2_Cd/H/Nd     H_OH        deltaHrxn(T=298K) = -13.548341132651473
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9765000e+01 5.1458000e+00 -8.9606000e-01 /
CHEB / 6.9118000e+00 2.4281000e+00 4.2961000e-01 /
CHEB / -6.4754000e+00 4.2830000e-01 3.1751000e-01 /
CHEB / -2.8315000e+00 -4.5994000e-01 1.3653000e-01 /
CHEB / -7.4872000e-01 -4.2017000e-01 4.6983000e-03 /

sC4H8O+HO2(+m)=sSPC(46)+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(370)) deltaHrxn(T=298K) = -5.929757691739987
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0091000e+01 -2.5434000e-01 -1.4631000e-01 /
CHEB / 1.7669000e+01 3.2440000e-01 1.7960000e-01 /
```

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CHEB / 5.3845000e-01 -2.6213000e-02 -3.1543000e-03 /
CHEB / 1.5933000e-01 -5.4491000e-02 -3.3151000e-02 /
CHEB / 7.2582000e-02 -6.0817000e-03 -8.6540000e-03 /

MEKenol+HO2(+m)=sSPC(46)+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(370)) deltaHrxn(T=298K) = 1.4995902230662281
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3713000e+01 -2.5043000e-01 -1.4601000e-01 /
CHEB / 1.9980000e+01 3.2044000e-01 1.7991000e-01 /
CHEB / 5.1006000e-01 -2.5943000e-02 -3.2604000e-03 /
CHEB / 1.4894000e-01 -5.4947000e-02 -3.3841000e-02 /
CHEB / 6.4874000e-02 -6.6182000e-03 -9.1384000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     C3H6O-enol  -37.48      71.5  19.4  23.83 27.67 30.87 35.79 39.39
      45.1  null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[OH]CHCH3+OH(+m)=C2H5O-2+C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (C4H10O2(377))  deltaHrxn(T=298K) = -
11.058946841085609 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0583000e+01 -1.2143000e+00 -9.3977000e-02 /
CHEB / 1.6105000e+00 1.0718000e+00 -2.5287000e-02 /
CHEB / 2.4917000e-01 3.4339000e-01 9.6065000e-02 /
CHEB / -1.4267000e-01 -5.8417000e-02 6.7241000e-02 /
CHEB / -1.1041000e-01 -1.2200000e-01 -3.8062000e-03 /

C2H5O-2+C2H5O-2(+m)=sC4H8O+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C4H10O2(377)) deltaHrxn(T=298K) = -71.22268175124512
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9954000e+00 -1.3723000e+00 -6.5414000e-02 /
CHEB / 2.2821000e+00 1.0045000e+00 -6.1308000e-02 /
CHEB / 4.2135000e-01 4.9027000e-01 4.5711000e-02 /
CHEB / -7.7429000e-02 6.8937000e-02 8.0408000e-02 /
CHEB / -8.9359000e-02 -1.0438000e-01 4.0563000e-02 /

CH3CH[OH]CHCH3+OH(+m)=sC4H8O+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (C4H10O2(377))  deltaHrxn(T=298K) = -
82.28162859233072 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5824000e+00 -1.2805000e+00 -8.8474000e-02 /
CHEB / 2.0069000e+00 1.0380000e+00 -4.1516000e-02 /
CHEB / 3.0699000e-01 4.0769000e-01 7.9537000e-02 /
CHEB / -7.9349000e-02 -1.0785000e-03 7.7997000e-02 /
CHEB / -8.8751000e-02 -1.1352000e-01 1.6148000e-02 /

C2H5O-2+C2H5O-2(+m)=MEKenol+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C4H10O2(377)) deltaHrxn(T=298K) = -78.65202966605133
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0481000e+01 -1.3923000e+00 -6.4980000e-02 /
CHEB / 1.4431000e+00 9.8364000e-01 -6.4612000e-02 /
CHEB / 1.6808000e-01 5.0169000e-01 3.9066000e-02 /
CHEB / -1.5147000e-01 9.2633000e-02 7.8455000e-02 /
CHEB / -1.2054000e-01 -9.0759000e-02 4.5179000e-02 /

CH3CH[OH]CHCH3+OH(+m)=MEKenol+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (C4H10O2(377))  deltaHrxn(T=298K) = -
89.71097650713693 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0896000e+01 -1.2975000e+00 -8.8371000e-02 /
CHEB / 1.3024000e+00 1.0246000e+00 -4.5832000e-02 /
CHEB / 6.9198000e-02 4.2090000e-01 7.5055000e-02 /
CHEB / -1.6034000e-01 1.6507000e-02 7.9713000e-02 /
CHEB / -1.2087000e-01 -1.0666000e-01 2.1437000e-02 /

sC4H8O+H2O(+m)=MEKenol+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C4H10O2(377)) deltaHrxn(T=298K) = -7.429347914806208
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4350000e+01 -1.5008000e+00 -4.9248000e-02 /
CHEB / 2.1713000e+01 8.6904000e-01 -6.8222000e-02 /
CHEB / 8.8253000e-01 5.5480000e-01 -2.7733000e-03 /
CHEB / -1.0147000e-01 2.1745000e-01 4.7382000e-02 /
CHEB / -1.8952000e-01 -1.0242000e-02 5.2905000e-02 /

C2H5O-2+C2H5O-2(+m)=CH3OH+C3H6O-enol(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (C4H10O2(377))  deltaHrxn(T=298K) = -
59.65351049979928 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 8.7442000e+00 -1.3566000e+00 -6.6209000e-02 /
CHEB / 2.3820000e+00 1.0194000e+00 -5.8910000e-02 /
CHEB / 4.5064000e-01 4.7905000e-01 5.1044000e-02 /
CHEB / -8.2723000e-02 5.0108000e-02 8.1425000e-02 /
CHEB / -8.8291000e-02 -1.1321000e-01 3.6346000e-02 /

CH3CH[OH]CHCH3+OH(+m)=CH3OH+C3H6O-enol(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #7 (C4H10O2(377)) deltaHrxn(T=298K)
= -70.7124573408849 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4764000e+00 -1.2669000e+00 -8.8934000e-02 /
CHEB / 1.9791000e+00 1.0474000e+00 -3.8217000e-02 /
CHEB / 3.3090000e-01 3.9587000e-01 8.3031000e-02 /
CHEB / -7.6627000e-02 -1.4665000e-02 7.6292000e-02 /
CHEB / -8.7800000e-02 -1.1760000e-01 1.1875000e-02 /

CH3OH+C3H6O-enol(+m)=sC4H8O+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C4H10O2(377)) deltaHrxn(T=298K) = -11.56917125144583
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2820000e+01 -1.4504000e+00 -5.3403000e-02 /
CHEB / 2.0336000e+01 9.3209000e-01 -6.6415000e-02 /
CHEB / 1.0140000e+00 5.4297000e-01 1.4387000e-02 /
CHEB / -6.5664000e-02 1.6005000e-01 6.4176000e-02 /
CHEB / -1.5333000e-01 -5.8946000e-02 5.3969000e-02 /

CH3OH+C3H6O-enol(+m)=MEKenol+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7 (C4H10O2(377))  deltaHrxn(T=298K) = -
18.998519166252045 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0921000e+01 -1.4765000e+00 -5.1818000e-02 /
CHEB / 1.9089000e+01 8.9969000e-01 -6.8139000e-02 /
CHEB / 7.7997000e-01 5.4972000e-01 5.5174000e-03 /
CHEB / -1.1367000e-01 1.9013000e-01 5.6296000e-02 /
CHEB / -1.8674000e-01 -3.4050000e-02 5.4395000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
```

```
!     C2H2              53.86 48.02 10.56 11.98 12.98 13.74 14.94 15.92
      17.7  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     C4H6-12           38.85 69.81 19.35 23.63 27.42 30.79 36.04 39.99
      46.09 null
!Here are the path reactions and their high-P limit kinetics:

C4H6-13+HO2(+m)=C4H6O(717)+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O2J(362)) deltaHrxn(T=298K) = -47.585416222840884
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1590000e+00 1.0967000e-04 6.8887000e-05 /
CHEB / 1.4117000e+01 2.9098000e-04 2.0697000e-04 /
CHEB / 1.8599000e-02 1.3099000e-04 9.6448000e-05 /
CHEB / -1.4571000e-01 -8.3317000e-05 -6.0748000e-05 /
CHEB / -1.4276000e-01 -1.7124000e-04 -1.2149000e-04 /

HO2+C4H6-12(+m)=C4H6O(717)+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O2J(362)) deltaHrxn(T=298K) = -60.35402450734764
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3019000e+00 -1.2409000e-05 -8.5956000e-06 /
CHEB / 1.2185000e+01 -1.7942000e-05 -1.2438000e-05 /
CHEB / 4.0453000e-01 -2.9412000e-06 -2.0587000e-06 /
CHEB / 1.3623000e-01 1.0506000e-05 7.2660000e-06 /
CHEB / 4.0920000e-02 1.5815000e-05 1.0969000e-05 /

HO2+C4H6-12(+m)=C4H6-13+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O2J(362)) deltaHrxn(T=298K) = -12.768608284506746
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9609000e+00 2.0653000e-04 1.4251000e-04 /
CHEB / 1.1284000e+01 3.3429000e-04 2.3226000e-04 /
CHEB / 2.6008000e-02 1.0746000e-04 7.5353000e-05 /
CHEB / -1.5300000e-01 -1.1002000e-04 -7.6511000e-05 /
CHEB / -1.4541000e-01 -2.1183000e-04 -1.4742000e-04 /

C4H6O(717)+OH(+m)=sSPC(46)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O2J(362)) deltaHrxn(T=298K) = 34.12682241748301
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9741000e+01 -2.2937000e-07 -1.6053000e-07 /
CHEB / 2.5901000e+01 -3.2338000e-07 -2.2615000e-07 /
CHEB / 3.3933000e-01 1.5834000e-09 1.4846000e-09 /
CHEB / 1.3238000e-01 3.3277000e-07 2.3287000e-07 /
CHEB / 5.4123000e-02 5.1240000e-07 3.5752000e-07 /

HO2+C4H6-12(+m)=sSPC(46)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O2J(362)) deltaHrxn(T=298K) = -26.227202089864623
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4151000e+00 -7.8095000e-04 -6.1495000e-04 /
CHEB / 3.8140000e+00 1.2020000e-03 9.4507000e-04 /
CHEB / 3.5355000e-01 -4.6093000e-04 -3.6140000e-04 /
CHEB / 1.2202000e-01 -1.5195000e-05 -1.3524000e-05 /
CHEB / 4.0652000e-02 8.7585000e-05 6.9180000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(116)+H(+m)=HO2+CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H10O3(339))  deltaHrxn(T=298K) = -
14.347966927396596 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1835000e+00 -1.7657000e-01 -1.0019000e-01 /
CHEB / 1.7220000e+00 2.3442000e-01 1.2924000e-01 /
CHEB / 4.8329000e-01 -4.0003000e-02 -1.6027000e-02 /
CHEB / 1.1560000e-01 -2.7090000e-02 -1.7612000e-02 /
CHEB / 2.6000000e-02 4.2475000e-03 8.8826000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
```

```
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(1013)  -47.63      104.06      35.2  42.15 48.1  52.8  60.33
      66.06 72.62 null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1013)+H(+m)=CH3CH[OH]CH2+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H10O3(723))  deltaHrxn(T=298K) = -
2.858994825165823 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7787000e+00 -5.4344000e-02 -3.5505000e-02 /
CHEB / 3.9899000e+00 7.4240000e-02 4.8086000e-02 /
CHEB / 1.0365000e+00 -1.6798000e-02 -1.0201000e-02 /
CHEB / 2.8553000e-01 -5.7521000e-03 -4.0996000e-03 /
CHEB / 8.6853000e-02 1.8694000e-03 1.1242000e-03 /

sSPC(1013)+H(+m)=CH3CH[OH]CH2CH2+HO2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H10O3(723))  deltaHrxn(T=298K) = -
22.366839259367627 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0386000e+01 -5.7211000e-02 -3.8600000e-02 /
CHEB / 1.3607000e+00 7.4048000e-02 4.9705000e-02 /
CHEB / 5.0477000e-01 -1.0019000e-02 -6.3304000e-03 /
CHEB / 1.8641000e-01 -9.4378000e-03 -6.4758000e-03 /
CHEB / 6.1261000e-02 9.4181000e-04 5.1050000e-04 /

CH3CH[OH]CH2+CH2OOH(+m)=CH3CH[OH]CH2CH2+HO2(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2 (C4H10O3(723)) deltaHrxn(T=298K)
= -19.507844434201804 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6158000e+00 -1.0026000e-01 -6.3605000e-02 /
CHEB / 1.3702000e+00 1.3122000e-01 8.2137000e-02 /
CHEB / 4.8285000e-01 -1.9834000e-02 -1.0683000e-02 /
CHEB / 9.5350000e-02 -1.5960000e-02 -1.0667000e-02 /
CHEB / 3.2258000e-04 1.9585000e-03 7.5047000e-04 /

sSPC(332)+H(+m)=sSPC(1013)+H(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H10O3(723)) deltaHrxn(T=298K) = 6.298996419490777
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -3.0122000e+00 -5.5276000e-02 -3.6102000e-02 /
CHEB / 4.6548000e+00 7.5373000e-02 4.8803000e-02 /
CHEB / 6.8931000e-01 -1.6799000e-02 -1.0188000e-02 /
CHEB / 1.5066000e-01 -6.0207000e-03 -4.2712000e-03 /
CHEB / 2.7528000e-02 1.8984000e-03 1.1349000e-03 /

sSPC(332)+H(+m)=CH3CH[OH]CH2+CH2OOH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H10O3(723))  deltaHrxn(T=298K) =
3.4400015943249542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0458000e+00 -7.6850000e-02 -4.8570000e-02 /
CHEB / 4.6652000e+00 1.0549000e-01 6.5790000e-02 /
CHEB / 9.7386000e-01 -2.4597000e-02 -1.3888000e-02 /
CHEB / 2.4157000e-01 -7.7901000e-03 -5.6947000e-03 /
CHEB / 6.6769000e-02 2.6057000e-03 1.4719000e-03 /

sSPC(332)+H(+m)=CH3CH[OH]CH2CH2+HO2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H10O3(723))  deltaHrxn(T=298K) = -
16.06784283987685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1076000e+00 -1.0791000e-01 -6.7677000e-02 /
CHEB / 1.5318000e+00 1.4137000e-01 8.7354000e-02 /
CHEB / 5.0599000e-01 -2.1586000e-02 -1.1283000e-02 /
CHEB / 1.4985000e-01 -1.7091000e-02 -1.1369000e-02 /
CHEB / 4.0878000e-02 2.1198000e-03 7.5224000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
```

```
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(46)+CH3CH[OH]CHCH3(+m)=C4H7-24+sSPC(116)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C8H16O3(377)) deltaHrxn(T=298K)
= -14.38863964099292 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9540000e+00 -7.4669000e-01 -1.7039000e-01 /
CHEB / 3.0643000e+00 8.8488000e-01 1.4593000e-01 /
CHEB / 4.8966000e-01 -2.6838000e-03 8.0937000e-02 /
CHEB / -2.9005000e-02 -1.3478000e-01 -3.2392000e-02 /
CHEB / -2.8866000e-02 -3.7019000e-02 -3.6858000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+CH3CH[OH]CHCH3(+m)=C4H7-24+sSPC(116)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #18 (C8H16O3(382))
      deltaHrxn(T=298K) = -15.958466467597553 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2610000e+00 -7.3865000e-01 -1.7335000e-01 /
CHEB / 2.9002000e+00 8.7244000e-01 1.5040000e-01 /
CHEB / 5.2884000e-01 1.9657000e-03 7.9134000e-02 /
CHEB / -5.9157000e-03 -1.3372000e-01 -3.2088000e-02 /
CHEB / -2.2125000e-02 -3.8470000e-02 -3.6739000e-02 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[OH]CH2CH2+sSPC(46)(+m)=sSPC(332)+C4H7-24(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #43 (C8H16O3(727))
      deltaHrxn(T=298K) = -12.668763728512673 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6948000e+00 -7.2233000e-01 -1.7026000e-01 /
CHEB / 3.1406000e+00 8.6752000e-01 1.5062000e-01 /
CHEB / 4.3380000e-01 -2.0405000e-02 7.5825000e-02 /
CHEB / -4.8248000e-02 -1.2827000e-01 -3.5615000e-02 /
CHEB / -4.2048000e-02 -3.0330000e-02 -3.3903000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
```

```
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[OH]CH2CH2+sSPC(56)(+m)=sSPC(332)+C4H7-24(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #78 (C8H16O3(728))
      deltaHrxn(T=298K) = -14.238590555117298 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8737000e+00 -7.1489000e-01 -1.7541000e-01 /
CHEB / 3.1018000e+00 8.4927000e-01 1.5634000e-01 /
CHEB / 4.6453000e-01 -7.2422000e-03 7.4212000e-02 /
CHEB / -2.7583000e-02 -1.2675000e-01 -3.3388000e-02 /
CHEB / -3.7062000e-02 -3.3888000e-02 -3.4018000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5              28.6  59.87 11.73 14.47 17.05 19.34 23.02 25.91
      31.53 null
!     C4H9-2            16.09 80.42 21.84 26.81 31.81 36.38 43.83 49.58
      59.02 null
!     CH3CH[O]C2H5      -18.47      82.48 26.0  32.47 38.36 43.0  50.56
      56.09 64.77 null
!     C4H8-1            -0.11 73.61 20.57 26.09 31.04 35.28 41.96 46.97
      54.75 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
```

```
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H8-2+sSPC(116)(+m)=C4H8-1+sSPC(116)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #131 (C8H17O3J(506))     deltaHrxn(T=298K) =
3.109740038709063 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9581000e+01 -8.4265000e-01 -1.3960000e-01 /
CHEB / 2.4298000e+01 1.0186000e+00 9.8155000e-02 /
CHEB / 1.0778000e+00 -2.1829000e-02 1.0462000e-01 /
CHEB / 1.3447000e-01 -1.6549000e-01 -3.4785000e-02 /
CHEB / 4.2232000e-02 -3.5066000e-02 -4.6706000e-02 /

sBuOH+sSPC(46)(+m)=C4H8-1+sSPC(116)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #131 (C8H17O3J(506))     deltaHrxn(T=298K) = -
1.0298701593073858 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8231000e+01 -8.5113000e-01 -1.3753000e-01 /
CHEB / 2.2828000e+01 1.0267000e+00 9.4369000e-02 /
CHEB / 1.0858000e+00 -1.8405000e-02 1.0619000e-01 /
CHEB / 1.4629000e-01 -1.6787000e-01 -3.3654000e-02 /
CHEB / 5.5623000e-02 -3.6535000e-02 -4.7597000e-02 /

C4H8-2+sSPC(116)(+m)=sBuOH+sSPC(46)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #131 (C8H17O3J(506))     deltaHrxn(T=298K) =
4.139610198016452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0179000e+01 -8.2748000e-01 -1.4304000e-01 /
CHEB / 2.4678000e+01 1.0043000e+00 1.0466000e-01 /
CHEB / 1.1159000e+00 -2.8154000e-02 1.0169000e-01 /
CHEB / 1.4516000e-01 -1.6119000e-01 -3.6746000e-02 /
CHEB / 4.4551000e-02 -3.2348000e-02 -4.5040000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CH[O]C2H5      -18.47      82.48 26.0  32.47 38.36 43.0  50.56
      56.09 64.77 null
!     C2H5              28.6  59.87 11.73 14.47 17.05 19.34 23.02 25.91
      31.53 null
!     C4H9-2            16.09 80.42 21.84 26.81 31.81 36.38 43.83 49.58
      59.02 null
```

```
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     C4H8-1            -0.11 73.61 20.57 26.09 31.04 35.28 41.96 46.97
      54.75 null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+sBuOH(+m)=sSPC(332)+C4H8-1(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #140 (C8H17O3J(523))     deltaHrxn(T=298K) =
1.769837278658632 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9056000e+01 -8.7427000e-01 -1.4491000e-01 /
CHEB / 2.3994000e+01 1.0225000e+00 9.1739000e-02 /
CHEB / 1.0868000e+00 1.7464000e-02 1.1422000e-01 /
CHEB / 9.5302000e-02 -1.5897000e-01 -2.4484000e-02 /
CHEB / -2.6125000e-03 -5.0662000e-02 -4.9448000e-02 /

sSPC(332)+C4H8-2(+m)=sSPC(56)+sBuOH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #140 (C8H17O3J(523))     deltaHrxn(T=298K) =
1.3399027600504354 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9740000e+01 -8.6182000e-01 -1.4788000e-01 /
CHEB / 2.4671000e+01 1.0115000e+00 9.7215000e-02 /
CHEB / 1.1159000e+00 1.1635000e-02 1.1214000e-01 /
CHEB / 1.2180000e-01 -1.5596000e-01 -2.6404000e-02 /
CHEB / 1.8182000e-02 -4.8208000e-02 -4.8328000e-02 /

sSPC(332)+C4H8-2(+m)=sSPC(332)+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #140 (C8H17O3J(523))     deltaHrxn(T=298K) =
3.1097400387090604 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9041000e+01 -8.8895000e-01 -1.4104000e-01 /
CHEB / 2.4077000e+01 1.0358000e+00 8.4920000e-02 /
CHEB / 1.0896000e+00 2.3902000e-02 1.1657000e-01 /
CHEB / 1.1519000e-01 -1.6247000e-01 -2.2201000e-02 /
CHEB / 1.8541000e-02 -5.3377000e-02 -5.0675000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H7-24          32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     CH3CH[o]C2H3     12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C4H6-13          26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H6-13+sSPC(116)(+m)=sC4H8O+sSPC(46)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #155 (C8H15O3J(547))     deltaHrxn(T=298K) =
6.019505019033584 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8794000e+01 -5.5742000e-01 -1.7900000e-01 /
CHEB / 2.3032000e+01 6.9723000e-01 1.8975000e-01 /
CHEB / 1.1384000e+00 -5.5555000e-02 3.7681000e-02 /
CHEB / 2.0430000e-01 -9.8043000e-02 -4.1958000e-02 /
CHEB / 5.6368000e-02 -1.1315000e-02 -2.0335000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CH[o]C2H3     12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H7-24          32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
```

```
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(332)+C4H6-13(+m)=sSPC(56)+sC4H8O(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #208 (C8H15O3J(597))     deltaHrxn(T=298K) =
3.21979758106756 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8593000e+01 -7.4431000e-01 -1.7645000e-01 /
CHEB / 2.3399000e+01 8.7957000e-01 1.4902000e-01 /
CHEB / 1.0412000e+00 -3.8725000e-03 8.6276000e-02 /
CHEB / 1.5071000e-01 -1.2673000e-01 -3.3476000e-02 /
CHEB / 2.7121000e-02 -3.8457000e-02 -3.7833000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     CH3CH[O]C2H5      -18.47      82.48 26.0  32.47 38.36 43.0  50.56
      56.09 64.77 null
!     C2H5              28.6  59.87 11.73 14.47 17.05 19.34 23.02 25.91
      31.53 null
!     C4H9-2            16.09 80.42 21.84 26.81 31.81 36.38 43.83 49.58
      59.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C4H8-1            -0.11 73.61 20.57 26.09 31.04 35.28 41.96 46.97
      54.75 null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:
```

```
CH3CH[OH]CHCH3+CH3CH[O]C2H5(+m)=MEKenol+sBuOH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #245 (C8H18O2(606))
      deltaHrxn(T=298K) = -74.55251756523559 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1865000e+00 -1.4649000e+00 -1.7123000e-02 /
CHEB / 4.6104000e+00 9.4519000e-01 -1.8720000e-02 /
CHEB / 5.9443000e-01 6.2664000e-01 1.3792000e-02 /
CHEB / -4.5482000e-01 2.5001000e-01 3.3954000e-02 /
CHEB / -4.2060000e-01 -4.8982000e-02 2.3739000e-02 /

CH3CH[OH]CHCH3+CH3CH[O]C2H5(+m)=sC4H8O+sBuOH(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #245 (C8H18O2(606))
      deltaHrxn(T=298K) = -67.12316965042938 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2982000e+00 -1.4643000e+00 -1.7871000e-02 /
CHEB / 5.1368000e+00 9.4540000e-01 -1.9700000e-02 /
CHEB / 7.1145000e-01 6.2525000e-01 1.3938000e-02 /
CHEB / -4.2123000e-01 2.4801000e-01 3.4954000e-02 /
CHEB / -4.0502000e-01 -4.9664000e-02 2.4753000e-02 /

sC4H8O+sBuOH(+m)=MEKenol+sBuOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #245 (C8H18O2(606))     deltaHrxn(T=298K) = -
7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6199000e+01 -1.4836000e+00 -9.2350000e-03 /
CHEB / 2.3316000e+01 9.2421000e-01 -1.0264000e-02 /
CHEB / 1.0161000e+00 6.4039000e-01 7.0382000e-03 /
CHEB / -3.8840000e-01 2.8573000e-01 1.8034000e-02 /
CHEB / -4.2965000e-01 -2.3108000e-02 1.2983000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H9O2J(53) -57.23      98.0  29.31 35.92 41.78 46.36 53.89 59.32
      65.89 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     C2H5O-1           -7.2  70.51 14.71 17.83 20.61 23.05 26.99 29.97
      32.69 null
!     C4H9O-2           -19.71      91.07 24.94 30.32 35.53 40.25 47.94
      53.75 61.21 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
```

```
!     C4H9O2J(54) -59.88      99.03 28.58 34.95 40.59 45.37 53.3  58.61
      65.35 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     C4H8O-enol3       -35.91      84.25 23.67 29.6  34.76 39.15 46.07
      51.14 56.94 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C4H8O-enol2       -37.68      83.04 23.93 29.26 34.16 38.51 45.56
      50.76 58.66 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!Here are the path reactions and their high-P limit kinetics:

C4H9O2J(53)+H(+m)=C2H5O-2+C2H5O-1(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
11.878375135909295 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1546000e+01 -1.2762000e+00 -6.7685000e-02 /
CHEB / 1.7096000e+00 1.0803000e+00 -3.8791000e-02 /
CHEB / 1.4661000e-01 4.1115000e-01 7.5447000e-02 /
CHEB / -1.8660000e-01 -2.8817000e-02 7.3647000e-02 /
CHEB / -1.1102000e-01 -1.3375000e-01 8.7919000e-03 /

C4H9O2J(53)+H(+m)=C4H9O-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
2.1595165669069214 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7739000e+00 -1.2304000e+00 -7.5940000e-02 /
CHEB / 3.3817000e+00 1.0962000e+00 -3.0184000e-02 /
CHEB / 4.2745000e-01 3.5816000e-01 8.8848000e-02 /
CHEB / -1.0015000e-01 -6.5139000e-02 6.6896000e-02 /
CHEB / -6.6704000e-02 -1.3021000e-01 -4.2156000e-03 /

C4H9O-2+OH(+m)=C2H5O-2+C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
9.718858569002371 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7852000e+00 -1.3025000e+00 -6.1352000e-02 /
CHEB / 2.0412000e+00 1.0711000e+00 -4.3131000e-02 /
CHEB / 1.1992000e-01 4.4047000e-01 6.5961000e-02 /
CHEB / -2.7768000e-01 -7.7677000e-03 7.5564000e-02 /
CHEB / -1.7139000e-01 -1.3493000e-01 1.6212000e-02 /

C4H9O2J(53)+H(+m)=CH3CH[OH]CH2+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
11.858293965488036 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1499000e+01 -1.2785000e+00 -6.7367000e-02 /
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CHEB / 2.3595000e+00 1.0792000e+00 -3.9137000e-02 /
CHEB / 3.2206000e-01 4.1373000e-01 7.4779000e-02 /
CHEB / -1.2374000e-01 -2.6620000e-02 7.3902000e-02 /
CHEB / -8.6834000e-02 -1.3367000e-01 9.4841000e-03 /

CH3CH[OH]CH2+CH2OH(+m)=C2H5O-2+C2H5O-1(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -0.020081170421259564 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7917000e+00 -1.3551000e+00 -5.1795000e-02 /
CHEB / 3.5175000e+00 1.0377000e+00 -4.7580000e-02 /
CHEB / 1.5847000e-01 4.9740000e-01 4.6324000e-02 /
CHEB / -3.4358000e-01 5.0725000e-02 7.4305000e-02 /
CHEB / -2.1365000e-01 -1.2576000e-01 3.1571000e-02 /

C4H9O-2+OH(+m)=CH3CH[OH]CH2+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
9.698777398581115 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7464000e+00 -1.3048000e+00 -6.1021000e-02 /
CHEB / 2.6829000e+00 1.0697000e+00 -4.3402000e-02 /
CHEB / 2.9684000e-01 4.4307000e-01 6.5201000e-02 /
CHEB / -2.1464000e-01 -5.2478000e-03 7.5688000e-02 /
CHEB / -1.4744000e-01 -1.3465000e-01 1.6936000e-02 /

C4H9O2J(53)+H(+m)=C4H9O2J(54)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
2.6496583597644303 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1357000e+00 -1.2229000e+00 -7.7613000e-02 /
CHEB / 2.4211000e+00 1.0974000e+00 -2.8396000e-02 /
CHEB / 1.4020000e-01 3.4971000e-01 9.0886000e-02 /
CHEB / -1.9940000e-01 -6.9557000e-02 6.5530000e-02 /
CHEB / -1.0473000e-01 -1.2898000e-01 -6.0745000e-03 /

C4H9O2J(54)+H(+m)=C2H5O-2+C2H5O-1(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
9.228716776144864 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0569000e+01 -1.2944000e+00 -6.3199000e-02 /
CHEB / 1.9822000e+00 1.0746000e+00 -4.1975000e-02 /
CHEB / 1.6361000e-01 4.3131000e-01 6.8976000e-02 /
CHEB / -2.0932000e-01 -1.4873000e-02 7.5134000e-02 /
CHEB / -1.2433000e-01 -1.3485000e-01 1.3847000e-02 /

C4H9O2J(54)+H(+m)=C4H9O-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) =
0.4901417928575089 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7046000e+00 -1.2477000e+00 -7.1689000e-02 /
CHEB / 3.7630000e+00 1.0937000e+00 -3.4312000e-02 /
CHEB / 4.1827000e-01 3.7727000e-01 8.3816000e-02 /
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CHEB / -1.2141000e-01 -5.5103000e-02 6.9732000e-02 /
CHEB / -7.7701000e-02 -1.3294000e-01 8.1085000e-05 /

C4H9O2J(54)+H(+m)=CH3CH[OH]CH2+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
9.208635605723606 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0527000e+01 -1.2967000e+00 -6.2872000e-02 /
CHEB / 2.6269000e+00 1.0732000e+00 -4.2271000e-02 /
CHEB / 3.3996000e-01 4.3392000e-01 6.8243000e-02 /
CHEB / -1.4633000e-01 -1.2458000e-02 7.5302000e-02 /
CHEB / -1.0029000e-01 -1.3464000e-01 1.4564000e-02 /

C4H9O2J(53)+H(+m)=CH3CH[OH]CH2CH2+OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
3.8794036518386132 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5912000e+00 -1.2440000e+00 -7.3142000e-02 /
CHEB / 3.5731000e+00 1.0930000e+00 -3.3111000e-02 /
CHEB / 5.3566000e-01 3.7373000e-01 8.4998000e-02 /
CHEB / -6.2379000e-02 -5.6076000e-02 6.9200000e-02 /
CHEB / -5.4328000e-02 -1.3209000e-01 -6.3247000e-04 /

CH3CH[OH]CH2CH2+OH(+m)=C2H5O-2+C2H5O-1(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -7.9989714840706805 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0675000e+01 -1.3173000e+00 -5.8262000e-02 /
CHEB / 2.3820000e+00 1.0637000e+00 -4.4844000e-02 /
CHEB / 1.4601000e-01 4.5701000e-01 6.0405000e-02 /
CHEB / -2.9440000e-01 6.4927000e-03 7.5927000e-02 /
CHEB / -1.8381000e-01 -1.3424000e-01 2.0586000e-02 /

CH3CH[OH]CH2CH2+OH(+m)=C4H9O-2+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) =
1.7198870849316918 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6598000e+00 -1.2694000e+00 -6.7020000e-02 /
CHEB / 4.3457000e+00 1.0874000e+00 -3.8477000e-02 /
CHEB / 3.5071000e-01 4.0220000e-01 7.6932000e-02 /
CHEB / -2.0132000e-01 -3.9288000e-02 7.2692000e-02 /
CHEB / -1.3413000e-01 -1.3533000e-01 6.1048000e-03 /

CH3CH[OH]CH2CH2+OH(+m)=CH3CH[OH]CH2+CH2OH(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -7.978890313649423 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0642000e+01 -1.3196000e+00 -5.7923000e-02 /
CHEB / 3.0174000e+00 1.0621000e+00 -4.5072000e-02 /
CHEB / 3.2434000e-01 4.5961000e-01 5.9599000e-02 /
CHEB / -2.3131000e-01 9.2101000e-03 7.5962000e-02 /
CHEB / -1.6003000e-01 -1.3382000e-01 2.1315000e-02 /
```

```
C4H9O2J(54)+H(+m)=CH3CH[OH]CH2CH2+OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
1.229745292074183 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5476000e+00 -1.2616000e+00 -6.8805000e-02 /
CHEB / 3.9230000e+00 1.0897000e+00 -3.6991000e-02 /
CHEB / 5.3527000e-01 3.9325000e-01 7.9522000e-02 /
CHEB / -8.4829000e-02 -4.5004000e-02 7.1721000e-02 /
CHEB / -6.5764000e-02 -1.3450000e-01 3.9238000e-03 /

C4H9O2J(53)+H(+m)=C4H8O-enol3+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
85.47102664426268 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1126000e+01 -1.3359000e+00 -6.2217000e-02 /
CHEB / 1.7954000e+00 1.0410000e+00 -4.7590000e-02 /
CHEB / 1.5901000e-01 4.7616000e-01 5.8687000e-02 /
CHEB / -1.4125000e-01 4.0964000e-02 7.9020000e-02 /
CHEB / -1.0385000e-01 -1.2028000e-01 2.8316000e-02 /

C2H5O-2+C2H5O-1(+m)=C4H8O-enol3+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
73.59265150835338 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8784000e+00 -1.4219000e+00 -4.5073000e-02 /
CHEB / 2.2918000e+00 9.7381000e-01 -5.0953000e-02 /
CHEB / 2.4750000e-01 5.5272000e-01 2.4511000e-02 /
CHEB / -2.4205000e-01 1.4536000e-01 6.4850000e-02 /
CHEB / -1.9615000e-01 -8.1000000e-02 4.6463000e-02 /

C4H9O-2+OH(+m)=C4H8O-enol3+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
83.31151007735575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5705000e+00 -1.3649000e+00 -5.5396000e-02 /
CHEB / 1.9333000e+00 1.0237000e+00 -5.0065000e-02 /
CHEB / 1.4561000e-01 5.0478000e-01 4.6842000e-02 /
CHEB / -2.2259000e-01 7.1487000e-02 7.6496000e-02 /
CHEB / -1.6867000e-01 -1.1324000e-01 3.5620000e-02 /

CH3CH[OH]CH2+CH2OH(+m)=C4H8O-enol3+H2O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -73.61273267877463 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3198000e+00 -1.4248000e+00 -4.4643000e-02 /
CHEB / 2.6225000e+00 9.7079000e-01 -5.0928000e-02 /
CHEB / 3.0596000e-01 5.5470000e-01 2.3458000e-02 /
CHEB / -2.5993000e-01 1.4944000e-01 6.4067000e-02 /
CHEB / -2.2605000e-01 -7.8613000e-02 4.6822000e-02 /
```

```
C4H9O2J(54)+H(+m)=C4H8O-enol3+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
82.82136828449825 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0283000e+01 -1.3559000e+00 -5.7396000e-02 /
CHEB / 1.9429000e+00 1.0297000e+00 -4.9496000e-02 /
CHEB / 1.8366000e-01 4.9603000e-01 5.0550000e-02 /
CHEB / -1.5769000e-01 6.1368000e-02 7.7543000e-02 /
CHEB / -1.2003000e-01 -1.1600000e-01 3.3408000e-02 /

CH3CH[OH]CH2CH2+OH(+m)=C4H8O-enol3+H2O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -81.59162299242405 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0612000e+01 -1.3813000e+00 -5.2013000e-02 /
CHEB / 2.1237000e+00 1.0112000e+00 -5.0720000e-02 /
CHEB / 1.8733000e-01 5.2016000e-01 4.0115000e-02 /
CHEB / -2.3199000e-01 9.1309000e-02 7.3972000e-02 /
CHEB / -1.8447000e-01 -1.0665000e-01 3.9402000e-02 /

C4H9O2J(53)+H(+m)=C4H8O-enol2+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
87.24086377042724 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1521000e+01 -1.3411000e+00 -6.2101000e-02 /
CHEB / 1.5373000e+00 1.0370000e+00 -4.8507000e-02 /
CHEB / 7.3583000e-02 4.8170000e-01 5.7360000e-02 /
CHEB / -1.6919000e-01 4.8191000e-02 7.9568000e-02 /
CHEB / -1.1556000e-01 -1.1804000e-01 3.0284000e-02 /

C2H5O-2+C2H5O-1(+m)=C4H8O-enol2+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
75.36248863451794 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3582000e+00 -1.4285000e+00 -4.4750000e-02 /
CHEB / 1.9654000e+00 9.6662000e-01 -5.1489000e-02 /
CHEB / 1.5947000e-01 5.5707000e-01 2.2486000e-02 /
CHEB / -2.6498000e-01 1.5534000e-01 6.3681000e-02 /
CHEB / -2.0814000e-01 -7.4562000e-02 4.7703000e-02 /

C4H9O-2+OH(+m)=C4H8O-enol2+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
85.08134720352031 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9857000e+00 -1.3705000e+00 -5.5207000e-02 /
CHEB / 1.6602000e+00 1.0187000e+00 -5.0841000e-02 /
CHEB / 5.9019000e-02 5.1014000e-01 4.5249000e-02 /
CHEB / -2.4970000e-01 7.9710000e-02 7.6512000e-02 /
CHEB / -1.8053000e-01 -1.0986000e-01 3.7476000e-02 /
```

```
CH3CH[OH]CH2+CH2OH(+m)=C4H8O-enol2+H2O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -75.3825698049392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8043000e+00 -1.4315000e+00 -4.4314000e-02 /
CHEB / 2.2920000e+00 9.6347000e-01 -5.1454000e-02 /
CHEB / 2.1798000e-01 5.5898000e-01 2.1416000e-02 /
CHEB / -2.8250000e-01 1.5948000e-01 6.2837000e-02 /
CHEB / -2.3803000e-01 -7.1995000e-02 4.8018000e-02 /

C4H9O2J(54)+H(+m)=C4H8O-enol2+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
84.59120541066281 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0691000e+01 -1.3614000e+00 -5.7229000e-02 /
CHEB / 1.6751000e+00 1.0251000e+00 -5.0315000e-02 /
CHEB / 9.7432000e-02 5.0147000e-01 4.9036000e-02 /
CHEB / -1.8512000e-01 6.9280000e-02 7.7733000e-02 /
CHEB / -1.3185000e-01 -1.1301000e-01 3.5314000e-02 /

CH3CH[OH]CH2CH2+OH(+m)=C4H8O-enol2+H2O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C4H10O2(697))
      deltaHrxn(T=298K) = -83.36146011858861 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1042000e+01 -1.3872000e+00 -5.1783000e-02 /
CHEB / 1.8394000e+00 1.0057000e+00 -5.1419000e-02 /
CHEB / 1.0010000e-01 5.2533000e-01 3.8384000e-02 /
CHEB / -2.5833000e-01 1.0009000e-01 7.3653000e-02 /
CHEB / -1.9641000e-01 -1.0250000e-01 4.1132000e-02 /

C4H8O-enol2+H2O(+m)=C4H8O-enol3+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) =
1.7698371261645605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6460000e+01 -1.5176000e+00 -3.5427000e-02 /
CHEB / 2.3547000e+01 8.5738000e-01 -5.0417000e-02 /
CHEB / 9.1190000e-01 5.8646000e-01 -4.0053000e-03 /
CHEB / -2.1275000e-01 2.7150000e-01 3.6534000e-02 /
CHEB / -2.9811000e-01 2.6326000e-02 4.8487000e-02 /

C4H9O2J(53)+H(+m)=sC4H8O+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
88.81069059625973 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0096000e+01 -1.3310000e+00 -6.2399000e-02 /
CHEB / 2.1315000e+00 1.0448000e+00 -4.6784000e-02 /
CHEB / 2.6057000e-01 4.7100000e-01 5.9965000e-02 /
CHEB / -1.0812000e-01 3.4338000e-02 7.8567000e-02 /
CHEB / -9.0200000e-02 -1.2229000e-01 2.6549000e-02 /
```

```
C2H5O-2+C2H5O-1(+m)=sC4H8O+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
76.93231546035044 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7711000e+00 -1.4157000e+00 -4.5435000e-02 /
CHEB / 2.6935000e+00 9.8035000e-01 -5.0529000e-02 /
CHEB / 3.4972000e-01 5.4859000e-01 2.6373000e-02 /
CHEB / -2.1380000e-01 1.3626000e-01 6.5911000e-02 /
CHEB / -1.8199000e-01 -8.6648000e-02 4.5326000e-02 /

C4H9O-2+OH(+m)=sC4H8O+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
86.6511740293528 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5223000e+00 -1.3596000e+00 -5.5639000e-02 /
CHEB / 2.2836000e+00 1.0283000e+00 -4.9397000e-02 /
CHEB / 2.4794000e-01 4.9978000e-01 4.8345000e-02 /
CHEB / -1.9031000e-01 6.3976000e-02 7.6507000e-02 /
CHEB / -1.5484000e-01 -1.1622000e-01 3.3943000e-02 /

CH3CH[OH]CH2+CH2OH(+m)=sC4H8O+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
76.9523966307717 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2081000e+00 -1.4186000e+00 -4.5012000e-02 /
CHEB / 3.0283000e+00 9.7744000e-01 -5.0514000e-02 /
CHEB / 4.0800000e-01 5.5064000e-01 2.5337000e-02 /
CHEB / -2.3202000e-01 1.4027000e-01 6.5181000e-02 /
CHEB / -2.1186000e-01 -8.4419000e-02 4.5724000e-02 /

C4H9O2J(54)+H(+m)=sC4H8O+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
86.1610322364953 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2412000e+00 -1.3507000e+00 -5.7620000e-02 /
CHEB / 2.2882000e+00 1.0341000e+00 -4.8785000e-02 /
CHEB / 2.8577000e-01 4.9096000e-01 5.1987000e-02 /
CHEB / -1.2509000e-01 5.4134000e-02 7.7402000e-02 /
CHEB / -1.0625000e-01 -1.1865000e-01 3.1690000e-02 /

CH3CH[OH]CH2CH2+OH(+m)=sC4H8O+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #270 (C4H10O2(697))      deltaHrxn(T=298K) = -
84.93128694442112 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5504000e+00 -1.3759000e+00 -5.2291000e-02 /
CHEB / 2.4848000e+00 1.0163000e+00 -5.0129000e-02 /
CHEB / 2.9000000e-01 5.1533000e-01 4.1733000e-02 /
CHEB / -2.0047000e-01 8.3298000e-02 7.4277000e-02 /
CHEB / -1.7054000e-01 -1.1031000e-01 3.7833000e-02 /
```

```
C4H8O-enol3+H2O(+m)=sC4H8O+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -
3.3396639519970606 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8161000e+01 -1.5000000e+00 -3.6599000e-02 /
CHEB / 2.4310000e+01 8.8125000e-01 -5.0345000e-02 /
CHEB / 9.9263000e-01 5.8532000e-01 3.6007000e-04 /
CHEB / -1.5808000e-01 2.5081000e-01 4.1720000e-02 /
CHEB / -2.4573000e-01 3.2622000e-03 4.9305000e-02 /

C4H8O-enol2+H2O(+m)=sC4H8O+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C4H10O2(697))     deltaHrxn(T=298K) = -1.5698268258325
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7897000e+01 -1.5089000e+00 -3.6059000e-02 /
CHEB / 2.4328000e+01 8.6927000e-01 -5.0488000e-02 /
CHEB / 9.3027000e-01 5.8623000e-01 -1.9191000e-03 /
CHEB / -1.9122000e-01 2.6161000e-01 3.9133000e-02 /
CHEB / -2.8250000e-01 1.4952000e-02 4.9051000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!Here are the path reactions and their high-P limit kinetics:
```

```
sC4H8O+CH3CH[OH]CHCH3(+m)=MEKenol+CH3CH[OH]CHCH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = -7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6809000e+01 -8.1422000e-01 -1.5960000e-01 /
CHEB / 2.1761000e+01 9.6654000e-01 1.2015000e-01 /
CHEB / 1.1262000e+00 -2.9142000e-03 1.0249000e-01 /
CHEB / 1.5456000e-01 -1.4858000e-01 -3.3212000e-02 /
CHEB / 4.1141000e-02 -4.2702000e-02 -4.5272000e-02 /

MEKenol+CH3CH[OH]CH2CH2(+m)=MEKenol+CH3CH[OH]CHCH3(+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = -2.6496583520903982 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1022000e+01 -1.6726000e+00 -3.0593000e-01 /
CHEB / 2.5828000e+01 1.9309000e+00 2.0994000e-01 /
CHEB / 1.1373000e+00 3.7605000e-02 2.0272000e-01 /
CHEB / 6.4191000e-03 -2.6648000e-01 -4.0773000e-02 /
CHEB / -4.1898000e-02 -9.1488000e-02 -7.7715000e-02 /

MEKenol+CH3CH[OH]CH2CH2(+m)=sC4H8O+CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = 4.7796895627158165 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1954000e+01 -1.6539000e+00 -3.0970000e-01 /
CHEB / 2.6421000e+01 1.9135000e+00 2.1731000e-01 /
CHEB / 1.2418000e+00 3.0960000e-02 1.9941000e-01 /
CHEB / 4.2904000e-02 -2.6286000e-01 -4.2829000e-02 /
CHEB / -2.8886000e-02 -8.8701000e-02 -7.6451000e-02 /

sC4H8O+CH3CH[OH]CH2CH2(+m)=MEKenol+CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = -10.079006266896613 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9130000e+01 -1.6480000e+00 -3.1113000e-01 /
CHEB / 2.3816000e+01 1.9072000e+00 2.1993000e-01 /
CHEB / 1.1755000e+00 2.9803000e-02 1.9821000e-01 /
CHEB / 2.5634000e-02 -2.6171000e-01 -4.3306000e-02 /
CHEB / -2.8634000e-02 -8.8073000e-02 -7.6047000e-02 /

sC4H8O+CH3CH[OH]CH2CH2(+m)=sC4H8O+CH3CH[OH]CHCH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = -2.6496583520903982 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0056000e+01 -1.6304000e+00 -3.1443000e-01 /
CHEB / 2.4403000e+01 1.8908000e+00 2.2662000e-01 /
CHEB / 1.2812000e+00 2.3462000e-02 1.9501000e-01 /
CHEB / 6.1862000e-02 -2.5829000e-01 -4.5194000e-02 /
CHEB / -1.5628000e-02 -8.5435000e-02 -7.4821000e-02 /
```

```
sC4H8O+CH3CH[OH]CH2CH2(+m)=MEKenol+CH3CH[OH]CH2CH2(+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #356 (C8H17O2J(588))
      deltaHrxn(T=298K) = -7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6832000e+01 -9.6546000e-01 -1.4253000e-01 /
CHEB / 2.2408000e+01 1.0489000e+00 6.0561000e-02 /
CHEB / 1.0400000e+00 1.0550000e-01 1.3019000e-01 /
CHEB / 2.3617000e-02 -1.4223000e-01 4.8102000e-03 /
CHEB / -4.5195000e-02 -7.7970000e-02 -4.8604000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sC4H8O+sSPC(116)(+m)=MEKenol+sSPC(116)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #442 (C8H17O4J(592))
      deltaHrxn(T=298K) = -7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7837000e+01 -9.7375000e-01 -1.4593000e-01 /
CHEB / 2.2643000e+01 1.0290000e+00 2.2701000e-02 /
CHEB / 9.5089000e-01 2.0461000e-02 1.2333000e-01 /
CHEB / 1.4293000e-01 -1.1747000e-01 1.2359000e-02 /
CHEB / 9.2544000e-02 2.0913000e-02 -2.1202000e-02 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sC4H8O+sSPC(332)(+m)=MEKenol+sSPC(332)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #481 (C8H17O4J(795))
      deltaHrxn(T=298K) = -7.429347914806208 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6948000e+01 -9.5568000e-01 -1.2568000e-01 /
CHEB / 2.2158000e+01 1.0840000e+00 5.5846000e-02 /
CHEB / 9.9365000e-01 6.7034000e-02 1.2469000e-01 /
CHEB / 8.0255000e-02 -1.7411000e-01 -7.7631000e-03 /
CHEB / 1.5156000e-02 -7.0433000e-02 -5.4760000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
```

```
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+C4H7-24(+m)=sSPC(46)+C4H7-24(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #538 (C8H14O2(411))      deltaHrxn(T=298K) = -
1.5698268266046256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8539000e+00 -8.3256000e-01 -1.4584000e-01 /
CHEB / 4.2169000e+00 9.8066000e-01 1.0495000e-01 /
CHEB / 4.0580000e-01 4.9460000e-03 9.6665000e-02 /
CHEB / -5.6606000e-02 -1.4943000e-01 -2.6099000e-02 /
CHEB / -2.8658000e-02 -4.3834000e-02 -4.0856000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3CHO            -39.18      63.13 13.22 15.71 18.22 20.47 24.22
      26.97 29.78 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
HO2+sC4H8O(+m)=HO2+MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #681 (C4H9O3J(352))     deltaHrxn(T=298K) = -
7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8582000e+00 -1.0576000e-01 -7.2097000e-02 /
CHEB / 1.1707000e+01 1.4440000e-01 9.7188000e-02 /
CHEB / -2.1244000e-01 -2.4791000e-02 -1.4373000e-02 /
CHEB / -3.5587000e-01 -2.5780000e-02 -1.8738000e-02 /
CHEB / -2.7724000e-01 6.7812000e-03 3.7962000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3CH[OH]CHCH3    -22.93      85.73 29.6  34.49 38.99 42.99 49.61
      54.76 63.12  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH3CH[OH]CHCH3=sSPC(116)   3.7700000e+12      0.00000
0.0000000e+00
!     sSPC(46)+H2O=sSPC(116)  6.5200000e+01      2.92000
5.0700000e+04
!     sSPC(116)=HO2+sC4H8O    8.8110000e+09      1.17000
3.0100000e+04
!     sSPC(116)=HO2+MEKenol   6.4800000e+10      0.57000
2.9900000e+04

O2+CH3CH[OH]CHCH3(+m)=sSPC(116)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(116)) High-P Limit: R_Recombination estimate:
```

```
(Average:) O2_birad     C_rad/H/NonDeC          deltaHrxn(T=298K) = -
36.04576228514299 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6461000e+00 1.5306000e+00 -2.0350000e-01 /
CHEB / -9.2707000e+00 2.0896000e+00 -1.3533000e-01 /
CHEB / -5.6779000e+00 5.4212000e-01 1.0149000e-01 /
CHEB / -2.4966000e+00 -3.0917000e-01 6.6481000e-02 /
CHEB / -6.2566000e-01 -3.4682000e-01 -3.5392000e-02 /

O2+CH3CH[OH]CHCH3(+m)=sSPC(46)+H2O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(116))     deltaHrxn(T=298K) = -
23.15734975249154 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6394000e-01 -2.6486000e-01 -1.4507000e-01 /
CHEB / 9.8905000e+00 3.3086000e-01 1.7366000e-01 /
CHEB / 2.5333000e-01 -2.2611000e-02 -2.6976000e-04 /
CHEB / 7.9794000e-02 -5.1465000e-02 -2.9653000e-02 /
CHEB / 3.3938000e-02 -5.6175000e-03 -7.6901000e-03 /

O2+CH3CH[OH]CHCH3(+m)=HO2+sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(116))     deltaHrxn(T=298K) = -
13.927903380567912 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1192000e+01 -1.0064000e+00 -9.3065000e-02 /
CHEB / 1.4898000e+00 1.1410000e+00 3.8237000e-02 /
CHEB / -8.9382000e-02 1.0928000e-01 1.1028000e-01 /
CHEB / -1.3357000e-01 -2.1403000e-01 -1.0349000e-02 /
CHEB / -2.0429000e-02 -1.1468000e-01 -6.4410000e-02 /

O2+CH3CH[OH]CHCH3(+m)=HO2+MEKenol(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(116))     deltaHrxn(T=298K) = -
21.357251295374127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0361000e+01 -1.0064000e+00 -9.3065000e-02 /
CHEB / 1.2159000e+00 1.1410000e+00 3.8237000e-02 /
CHEB / -1.6138000e-01 1.0928000e-01 1.1028000e-01 /
CHEB / -1.5879000e-01 -2.1403000e-01 -1.0349000e-02 /
CHEB / -3.0357000e-02 -1.1468000e-01 -6.4410000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
```

```
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+C4H7-24=sSPC(46)     3.7700000e+12      0.00000
0.0000000e+00
!     sSPC(46)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04
!     sSPC(46)=HO2+C4H6-13    4.3669559e+09      1.31333
2.9866667e+04
!     CH3CH[o]C2H3+O=sSPC(46) 1.0000000e+13      0.00000
0.0000000e+00

O2+C4H7-24(+m)=sSPC(46)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H/OneDeC          deltaHrxn(T=298K) = -
22.40773737061649 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0327000e+01 1.1996000e+00 -1.5386000e-01 /
CHEB / -5.1625000e+00 8.1934000e-01 1.4552000e-01 /
CHEB / -2.7473000e+00 1.4119000e-01 3.0981000e-02 /
CHEB / -1.3174000e+00 -1.4197000e-01 -2.0424000e-02 /
CHEB / -5.1887000e-01 -1.0483000e-01 -2.4856000e-02 /

HO2+C4H6-12(+m)=O2+C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46))     deltaHrxn(T=298K) = -8.579077615449485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0806000e+01 -1.6103000e-01 -9.4903000e-02 /
CHEB / -6.0396000e-02 2.0807000e-01 1.2084000e-01 /
CHEB / 1.8520000e-01 -2.3049000e-02 -1.1272000e-02 /
CHEB / 1.6590000e-03 -3.3546000e-02 -1.8865000e-02 /
CHEB / -2.6644000e-02 2.8909000e-03 -6.6500000e-05 /

HO2+C4H6-13(+m)=sSPC(46)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46))     deltaHrxn(T=298K) = -18.968173409065525
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7131000e+00 2.9249000e+00 -3.4278000e-01 /
CHEB / -3.7747000e-01 3.2267000e-01 2.1552000e-01 /
CHEB / -2.4794000e+00 1.2773000e-02 7.5349000e-02 /
CHEB / -1.1830000e+00 -1.5317000e-01 -2.5597000e-02 /
CHEB / -4.4881000e-01 -1.0343000e-01 -3.1030000e-02 /
```

```
O2+C4H7-24(+m)=HO2+C4H6-13(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46))     deltaHrxn(T=298K) = -3.43956396155097
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2816000e+00 -1.6103000e-01 -9.4903000e-02 /
CHEB / 3.1189000e+00 2.0807000e-01 1.2084000e-01 /
CHEB / 2.2410000e-01 -2.3049000e-02 -1.1272000e-02 /
CHEB / 5.1890000e-03 -3.3546000e-02 -1.8865000e-02 /
CHEB / -2.6642000e-02 2.8909000e-03 -6.6500000e-05 /

CH3CH[o]C2H3+O(+m)=O2+C4H7-24(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46))     deltaHrxn(T=298K) = -36.88610511659995
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3228000e+01 5.0871000e-06 3.5358000e-06 /
CHEB / -4.3124000e-01 4.7206000e-06 3.2931000e-06 /
CHEB / -1.4174000e-01 -1.8453000e-06 -1.2803000e-06 /
CHEB / -9.8217000e-02 -4.0463000e-06 -2.8228000e-06 /
CHEB / -6.6168000e-02 -3.0243000e-06 -2.1089000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH2C[O]CH3  -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17 41.25
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     sSPC(1590)  -30.7 78.33 21.08 25.77 29.92 33.34 38.35 41.79 46.82
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH2C[O]CH3=sSPC(1356)      2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+CH3CO=sSPC(1356)    1.4157154e+13      -0.15000
2.9166667e+02
!     sSPC(1356)=tSPC(3683)   1.1250000e+11      0.00000
2.4400000e+04
!     sSPC(1590)+O=sSPC(1356) 1.0000000e+13      0.00000
0.0000000e+00
```

```
O2+CH2C[O]CH3(+m)=sSPC(1356)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/CO       deltaHrxn(T=298K) = -
25.317490786886196 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9740000e+00 1.1518000e+00 -1.3644000e-01 /
CHEB / -3.9877000e+00 8.4453000e-01 1.2082000e-01 /
CHEB / -2.2900000e+00 1.6935000e-01 3.8433000e-02 /
CHEB / -1.1436000e+00 -8.5376000e-02 -3.6207000e-03 /
CHEB / -4.8248000e-01 -8.2595000e-02 -1.4357000e-02 /

nSPC(102)+CH3CO(+m)=sSPC(1356)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     CO_rad/NonDe          deltaHrxn(T=298K) = -
79.94191189074998 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3255000e+00 5.7714000e+00 9.5807000e-01 /
CHEB / -3.7976000e+00 6.4780000e-01 1.7996000e-01 /
CHEB / -2.2560000e+00 4.8033000e-02 3.0601000e-02 /
CHEB / -1.0913000e+00 -6.4663000e-02 -4.6587000e-03 /
CHEB / -4.5504000e-01 -5.3936000e-02 -1.0580000e-02 /

nSPC(102)+CH3CO(+m)=O2+CH2C[O]CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1356))    deltaHrxn(T=298K) = -
54.62442110386379 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3107000e+01 3.2555000e-07 2.2661000e-07 /
CHEB / -4.3125000e-01 5.5770000e-07 3.8820000e-07 /
CHEB / -5.5728000e-02 3.7314000e-07 2.5973000e-07 /
CHEB / -2.8628000e-02 1.9703000e-07 1.3715000e-07 /
CHEB / -2.6270000e-02 7.2543000e-08 5.0495000e-08 /

sSPC(1590)+O(+m)=sSPC(1356)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/NonDe     Oa       deltaHrxn(T=298K) = -
59.72387148963201 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3893000e-01 5.5033000e+00 7.7979000e-01 /
CHEB / -3.7520000e+00 4.5759000e-01 5.9678000e-02 /
CHEB / -2.2787000e+00 -1.9798000e-02 -9.3684000e-03 /
CHEB / -1.1022000e+00 -9.2119000e-02 -1.9760000e-02 /
CHEB / -4.5107000e-01 -6.6408000e-02 -1.7116000e-02 /

sSPC(1590)+O(+m)=O2+CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356))   deltaHrxn(T=298K) = -34.406380702745814
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3246000e+01 2.1025000e-07 1.3921000e-07 /
CHEB / -2.2438000e-01 4.6814000e-07 3.3185000e-07 /
CHEB / -1.3304000e-02 2.6674000e-07 1.8993000e-07 /
CHEB / -1.0854000e-02 7.5041000e-08 4.9834000e-08 /
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CHEB / -7.7607000e-03 9.7522000e-09 5.1262000e-09 /

sSPC(1590)+O(+m)=nSPC(102)+CH3CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1356))    deltaHrxn(T=298K) =
20.218040401117968 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9337000e+00 -3.0672000e-04 -2.1349000e-04 /
CHEB / 7.9110000e+00 2.5083000e-04 1.7459000e-04 /
CHEB / 4.2098000e-01 9.5468000e-05 6.6448000e-05 /
CHEB / 1.2093000e-01 -1.7869000e-05 -1.2436000e-05 /
CHEB / 2.0085000e-02 -2.1205000e-05 -1.4759000e-05 /

sSPC(1356)(+m)=tSPC(3683)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356)) High-P Limit: intra_H_migration exact:
R5H_SSSS     O_rad_out     Cs_H_out_2H          deltaHrxn(T=298K) =
9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.5821000e-01 7.8912000e-01 -3.5503000e-02 /
CHEB / 4.2248000e+00 8.8992000e-01 3.5887000e-02 /
CHEB / -2.2467000e+00 1.7962000e-01 4.7407000e-02 /
CHEB / -1.1498000e+00 -7.7052000e-02 2.4802000e-03 /
CHEB / -4.8733000e-01 -8.1043000e-02 -1.5094000e-02 /

O2+CH2C[O]CH3(+m)=tSPC(3683)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356))   deltaHrxn(T=298K) = -15.698624026698795
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0890000e+00 -5.4525000e-01 -1.2760000e-01 /
CHEB / 5.9979000e-01 6.7902000e-01 1.3557000e-01 /
CHEB / 4.2838000e-02 -5.8638000e-02 2.0088000e-02 /
CHEB / 1.4056000e-02 -8.1958000e-02 -2.0577000e-02 /
CHEB / 2.5675000e-02 -1.2253000e-02 -1.3016000e-02 /

nSPC(102)+CH3CO(+m)=tSPC(3683)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356))   deltaHrxn(T=298K) = -70.32304513056258
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4862000e+00 1.6842000e-05 1.1727000e-05 /
CHEB / 2.9613000e-01 -9.3541000e-06 -6.5137000e-06 /
CHEB / 1.2500000e-01 -6.4966000e-06 -4.5242000e-06 /
CHEB / 3.3438000e-02 -6.2041000e-07 -4.3175000e-07 /
CHEB / -1.5663000e-03 9.0361000e-07 6.2952000e-07 /

sSPC(1590)+O(+m)=tSPC(3683)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1356))   deltaHrxn(T=298K) = -50.10500472944461
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6837000e+00 1.4426000e-04 1.0076000e-04 /
CHEB / 4.7302000e-01 -1.1893000e-04 -8.3095000e-05 /
CHEB / 1.5597000e-01 -4.6956000e-05 -3.2815000e-05 /
CHEB / 4.8062000e-02 9.9151000e-06 6.9675000e-06 /
CHEB / 1.6355000e-02 1.1556000e-05 8.0875000e-06 /
```

```
!PDepNetwork sSPC(1013) && sSPC(332)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     sSPC(1013)  -47.63      104.06      35.2  42.15 48.1  52.8  60.33
      66.06 72.62 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3CH[OH]CH2CH2   -21.44      85.19 28.95 34.38 39.34 43.58 50.3
      55.39 63.54  !MRH
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3CH[OH]CH2      -14.14      76.56 22.67 26.97 30.74 33.91 38.93
      42.77 49.05
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H2CCCH3[OH] -39.44      69.6  20.59 25.3  29.06 32.04 36.55 39.89
      45.32
!     sSPC(1072)  -76.48      99.01 32.08 38.74 44.26 48.98 56.59 62.32
      67.82 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH3CH[OH]CH2CH2=sSPC(332)  2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+CH3CH[OH]CH2=sSPC(332)    1.1500000e+13      0.00000
0.0000000e+00
!     sSPC(56)+H2O=sSPC(332)  1.1691492e+02      2.87714
4.8857143e+04
!     sSPC(332)=sSPC(1013)    2.2349237e+07      1.07833
1.8418333e+04
!     CH2OOH+H2CCCH3[OH]=sSPC(1013) 2.4100000e+10      0.00000
6.9600000e+03
```

```
!     sSPC(1072)+H=sSPC(1013) 2.3501400e+11      0.30815
4.9629937e+03
!     sSPC(332)=HO2+sC4H8O    1.9160000e+08      1.46000
2.9400000e+04

sSPC(1013)(+m)=sSPC(332)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -6.298996419490777
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0482000e-04 6.0689000e-01 -2.6774000e-02 /
CHEB / -4.8470000e+00 7.4430000e-01 -6.5476000e-03 /
CHEB / -6.0507000e+00 -1.7713000e-01 3.6310000e-02 /
CHEB / -2.9606000e+00 -7.2094000e-01 -1.0409000e-02 /
CHEB / -8.2931000e-01 -5.6805000e-01 -7.2485000e-02 /

O2+CH3CH[OH]CH2CH2(+m)=sSPC(332)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/Cs       deltaHrxn(T=298K) = -
33.16620773575839 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1795000e+00 1.0916000e+00 -1.0481000e-01 /
CHEB / -7.6394000e+00 1.6577000e+00 -1.1817000e-01 /
CHEB / -5.1292000e+00 5.9481000e-01 1.2910000e-02 /
CHEB / -2.5532000e+00 -1.9153000e-01 4.4965000e-02 /
CHEB / -8.2359000e-01 -3.5060000e-01 5.1206000e-03 /

O2+CH3CH[OH]CH2CH2(+m)=sSPC(1013)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
26.86721131626761 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2520000e+00 1.6906000e-02 -2.9297000e-01 /
CHEB / -4.2897000e+00 2.5603000e+00 -1.2192000e-01 /
CHEB / -4.0448000e+00 6.8565000e-01 9.4900000e-02 /
CHEB / -2.4666000e+00 -3.5369000e-01 3.1113000e-02 /
CHEB / -1.0517000e+00 -4.7362000e-01 -4.9111000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=sSPC(332)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     C_rad/H2/Cs           deltaHrxn(T=298K) = -
90.89043256578296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8837000e-01 1.0405000e+01 -1.3439000e+00 /
CHEB / -1.0729000e+01 8.4382000e-01 6.6703000e-01 /
CHEB / -6.1532000e+00 -4.2349000e-01 3.2833000e-01 /
CHEB / -2.8231000e+00 -6.6898000e-01 6.2455000e-02 /
CHEB / -9.2065000e-01 -3.8934000e-01 -6.3939000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=sSPC(1013)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
84.59143614629218 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0286000e-01 1.0253000e+01 -1.7276000e+00 /
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CHEB / -8.2400000e+00 1.1299000e+00 9.8665000e-01 /
CHEB / -4.9984000e+00 -3.6452000e-01 4.0123000e-01 /
CHEB / -2.5429000e+00 -6.1335000e-01 4.7468000e-02 /
CHEB / -1.0417000e+00 -3.5485000e-01 -7.8388000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=O2+CH3CH[OH]CH2CH2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K)
= -57.72422483002458 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3141000e+01 -5.3655000e-02 -4.2467000e-02 /
CHEB / -3.2233000e-01 7.1091000e-02 5.5820000e-02 /
CHEB / -1.3983000e-01 -1.1069000e-02 -7.8796000e-03 /
CHEB / -7.2081000e-02 -9.5016000e-03 -7.9172000e-03 /
CHEB / -4.8770000e-02 1.0006000e-03 5.9854000e-04 /

sSPC(332)(+m)=sSPC(56)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = 10.088705094685423
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8129000e+01 3.5544000e+00 -8.2874000e-01 /
CHEB / 1.0880000e+01 2.6422000e+00 5.1686000e-02 /
CHEB / -5.7785000e+00 4.7375000e-01 1.6878000e-01 /
CHEB / -2.7124000e+00 -4.3294000e-01 5.7517000e-02 /
CHEB / -8.3107000e-01 -4.4166000e-01 -2.8214000e-02 /

sSPC(1013)(+m)=sSPC(56)+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = 3.789708675194646
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6378000e+01 3.0018000e+00 -1.1590000e+00 /
CHEB / 1.1299000e+01 3.1729000e+00 2.1930000e-01 /
CHEB / -4.7044000e+00 5.3317000e-01 2.2327000e-01 /
CHEB / -2.5072000e+00 -4.6132000e-01 2.4873000e-02 /
CHEB / -9.9140000e-01 -4.6602000e-01 -6.2437000e-02 /

O2+CH3CH[OH]CH2CH2(+m)=sSPC(56)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
23.077502641072968 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5314000e-02 -5.7652000e-01 -2.0330000e-01 /
CHEB / 9.9667000e+00 6.8177000e-01 2.0623000e-01 /
CHEB / 1.2304000e-01 4.0768000e-03 5.3091000e-02 /
CHEB / -3.2154000e-02 -1.0404000e-01 -3.9376000e-02 /
CHEB / -2.4625000e-02 -3.8197000e-02 -3.2122000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=sSPC(56)+H2O(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K)
= -80.80172747109754 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1765000e+00 -1.0634000e-01 -6.8954000e-02 /
CHEB / 2.0656000e+00 1.3311000e-01 8.5043000e-02 /
CHEB / 6.2800000e-01 -1.2735000e-02 -6.1468000e-03 /
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CHEB / 1.6361000e-01 -1.6633000e-02 -1.1329000e-02 /
CHEB / 2.0263000e-02 -7.8392000e-04 -1.0234000e-03 /

CH2OOH+H2CCCH3[OH](+m)=sSPC(332)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
29.49667226818353 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6858000e+00 6.2381000e-02 -3.2219000e-01 /
CHEB / -4.4297000e+00 2.6073000e+00 -1.5238000e-01 /
CHEB / -5.0134000e+00 7.1716000e-01 7.9607000e-02 /
CHEB / -2.6461000e+00 -3.6728000e-01 4.0202000e-02 /
CHEB / -8.9343000e-01 -4.9755000e-01 -4.1053000e-02 /

CH2OOH+H2CCCH3[OH](+m)=sSPC(1013)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_rad/H2/O     Cd/H2_Cd/Nd2      deltaHrxn(T=298K)
= -23.197675848692754 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3157000e+00 1.4176000e+00 -3.0129000e-01 /
CHEB / -3.5906000e+00 1.5568000e+00 -8.1610000e-02 /
CHEB / -3.9126000e+00 4.3741000e-01 4.6483000e-02 /
CHEB / -2.1755000e+00 -1.4969000e-01 1.1283000e-02 /
CHEB / -9.0932000e-01 -2.6863000e-01 -8.6139000e-03 /

O2+CH3CH[OH]CH2CH2(+m)=CH2OOH+H2CCCH3[OH](+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K)
= -3.6695354675748604 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4777000e+00 -2.0412000e+00 -2.2285000e-01 /
CHEB / 3.2634000e+00 2.1567000e+00 9.9240000e-02 /
CHEB / -7.1618000e-01 3.7029000e-01 2.0656000e-01 /
CHEB / -7.3730000e-01 -3.2705000e-01 1.1536000e-02 /
CHEB / -3.5756000e-01 -2.8506000e-01 -9.6948000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=CH2OOH+H2CCCH3[OH](+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K)
= -61.393760297599435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9863000e+00 -8.6151000e-02 -9.1862000e-02 /
CHEB / -2.2979000e-01 1.3757000e-01 1.3261000e-01 /
CHEB / -3.4807000e-01 -3.7680000e-02 -2.3824000e-02 /
CHEB / -1.6232000e-01 -2.8737000e-02 -2.6987000e-02 /
CHEB / -6.6216000e-02 3.3484000e-03 -6.1820000e-04 /

CH2OOH+H2CCCH3[OH](+m)=sSPC(56)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
19.407967173498108 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5893000e+00 -1.2404000e+00 -4.0946000e-01 /
CHEB / 1.1253000e+01 1.4177000e+00 3.9711000e-01 /
CHEB / -3.7491000e-01 7.7560000e-02 1.2885000e-01 /
CHEB / -3.4651000e-01 -2.0594000e-01 -6.6274000e-02 /
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CHEB / -1.3200000e-01 -1.1535000e-01 -7.4008000e-02 /

sSPC(1072)+H(+m)=sSPC(332)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -29.546315208281868
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4056000e+00 -6.9362000e-02 -2.8167000e-01 /
CHEB / -4.6803000e+00 2.5116000e+00 -1.4735000e-01 /
CHEB / -4.8787000e+00 6.9823000e-01 7.5429000e-02 /
CHEB / -2.5991000e+00 -3.6308000e-01 3.7900000e-02 /
CHEB / -8.6864000e-01 -4.9339000e-01 -4.1293000e-02 /

sSPC(1072)+H(+m)=sSPC(1013)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
23.24731878879109 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1419000e+00 1.2743000e+00 -2.5448000e-01 /
CHEB / -3.9631000e+00 1.4852000e+00 -9.2029000e-02 /
CHEB / -3.7772000e+00 4.0833000e-01 5.1134000e-02 /
CHEB / -2.1073000e+00 -1.5476000e-01 1.4624000e-02 /
CHEB / -8.7991000e-01 -2.5561000e-01 -1.4458000e-02 /

sSPC(1072)+H(+m)=O2+CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) =
3.6198925274765195 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9309000e+00 -2.0717000e+00 -2.1294000e-01 /
CHEB / 4.2023000e+00 2.1755000e+00 8.7761000e-02 /
CHEB / -7.8054000e-01 3.9496000e-01 2.0278000e-01 /
CHEB / -7.6604000e-01 -3.3105000e-01 1.6173000e-02 /
CHEB / -3.5774000e-01 -2.9986000e-01 -9.4569000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=sSPC(1072)+H(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K)
= -61.3441173575011 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5428000e+00 -7.0586000e-02 -8.5197000e-02 /
CHEB / 4.4617000e-02 1.2400000e-01 1.2831000e-01 /
CHEB / -2.9140000e-01 -4.1103000e-02 -2.6237000e-02 /
CHEB / -1.4341000e-01 -2.9230000e-02 -2.8307000e-02 /
CHEB / -5.7783000e-02 3.6410000e-03 -8.2314000e-04 /

sSPC(1072)+H(+m)=sSPC(56)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -19.457610113596445
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3917000e+00 -1.2300000e+00 -4.1187000e-01 /
CHEB / 1.1327000e+01 1.4142000e+00 4.0437000e-01 /
CHEB / -3.7011000e-01 7.8743000e-02 1.2909000e-01 /
CHEB / -3.3564000e-01 -2.1392000e-01 -7.0646000e-02 /
CHEB / -1.1836000e-01 -1.2382000e-01 -7.8791000e-02 /
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sSPC(1072)+H(+m)=CH2OOH+H2CCCH3[OH](+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
0.04964294009833736 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3835000e+00 -1.0039000e+00 -1.4796000e-01 /
CHEB / 4.2142000e+00 1.0029000e+00 6.6614000e-02 /
CHEB / -2.7355000e-01 2.0465000e-01 1.1445000e-01 /
CHEB / -4.2652000e-01 -1.0286000e-01 2.0293000e-02 /
CHEB / -2.1189000e-01 -1.1887000e-01 -3.5260000e-02 /

HO2+sC4H8O(+m)=sSPC(332)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -17.748324640004427
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1125000e+00 9.2174000e-01 -6.9623000e-02 /
CHEB / -2.2050000e+00 1.4223000e+00 -8.3022000e-02 /
CHEB / -4.5785000e+00 5.2994000e-01 5.0453000e-03 /
CHEB / -2.3742000e+00 -1.6788000e-01 3.1371000e-02 /
CHEB / -7.6431000e-01 -3.2487000e-01 4.8210000e-03 /

HO2+sC4H8O(+m)=sSPC(1013)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -11.44932822051365
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5867000e-02 -2.2915000e-01 -2.2070000e-01 /
CHEB / 1.3744000e+00 2.3733000e+00 -1.1623000e-01 /
CHEB / -3.5359000e+00 6.4988000e-01 8.4923000e-02 /
CHEB / -2.3304000e+00 -3.5244000e-01 3.0735000e-02 /
CHEB / -1.0054000e+00 -4.7145000e-01 -4.7657000e-02 /

O2+CH3CH[OH]CH2CH2(+m)=HO2+sC4H8O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
15.417883095753961 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6081000e+00 -1.1396000e+00 -5.2800000e-02 /
CHEB / 2.6163000e+00 1.1832000e+00 -2.0918000e-03 /
CHEB / -8.1335000e-02 2.6898000e-01 8.0630000e-02 /
CHEB / -2.6091000e-01 -2.1196000e-01 2.0667000e-02 /
CHEB / -9.5899000e-02 -1.9960000e-01 -4.7338000e-02 /

nSPC(102)+CH3CH[OH]CH2(+m)=HO2+sC4H8O(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
73.14210792577853 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1781000e+01 -4.0701000e-02 -3.5492000e-02 /
CHEB / 6.4157000e-01 5.7071000e-02 4.8887000e-02 /
CHEB / 8.6432000e-02 -1.2186000e-02 -9.2260000e-03 /
CHEB / 7.8184000e-03 -7.9365000e-03 -7.2158000e-03 /
CHEB / -1.4820000e-02 1.8061000e-03 1.2340000e-03 /
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HO2+sC4H8O(+m)=sSPC(56)+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -7.6596195453190035
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3392000e+00 -5.6454000e-01 -2.0605000e-01 /
CHEB / 1.6203000e+01 6.7513000e-01 2.1467000e-01 /
CHEB / 3.7500000e-01 4.2526000e-03 5.2210000e-02 /
CHEB / 5.3898000e-02 -1.1105000e-01 -4.4896000e-02 /
CHEB / 1.7148000e-02 -4.4955000e-02 -3.6864000e-02 /

CH2OOH+H2CCCH3[OH](+m)=HO2+sC4H8O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (sSPC(332))     deltaHrxn(T=298K) = -
11.748347628179104 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8186000e+00 -2.0865000e+00 -2.0896000e-01 /
CHEB / 4.8209000e+00 2.1857000e+00 8.2866000e-02 /
CHEB / -5.9548000e-01 4.1371000e-01 1.9980000e-01 /
CHEB / -7.2687000e-01 -3.3839000e-01 1.9917000e-02 /
CHEB / -3.6310000e-01 -3.1649000e-01 -9.2797000e-02 /

sSPC(1072)+H(+m)=HO2+sC4H8O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(332))    deltaHrxn(T=298K) = -11.797990568277442
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2821000e+00 -2.1235000e+00 -1.9706000e-01 /
CHEB / 4.6442000e+00 2.2050000e+00 6.8435000e-02 /
CHEB / -5.5276000e-01 4.4188000e-01 1.9480000e-01 /
CHEB / -7.2467000e-01 -3.3844000e-01 2.5330000e-02 /
CHEB / -3.5544000e-01 -3.3052000e-01 -8.8406000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
```

```
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

sSPC(46)+sSPC(332)(+m)=sSPC(116)+sSPC(56)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C8H16O5JJ(385))
      deltaHrxn(T=298K) = -2.7997074379660276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8309000e+01 -3.1016000e-01 -1.4473000e-01 /
CHEB / 2.2299000e+01 4.0595000e-01 1.7850000e-01 /
CHEB / 1.3793000e+00 -5.6578000e-02 -7.3086000e-03 /
CHEB / 2.6930000e-01 -5.5779000e-02 -3.1514000e-02 /
CHEB / 5.9152000e-02 4.1278000e-03 -3.4799000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H7-24          32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3CH[o]C2H3     12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C4H6-13          26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     CH3C[OH]CHcH2    -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!Here are the path reactions and their high-P limit kinetics:

C4H6-13+CH3C[OH]CHcH2(+m)=C4H7-24+C4H6O(717)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #22 (C8H13OJ(507))
      deltaHrxn(T=298K) = -13.01850572483287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.1203000e+00 4.0981000e-10 2.8526000e-10 /
CHEB / 1.7245000e+01 8.0060000e-10 5.5728000e-10 /
CHEB / 3.4144000e-01 7.4545000e-10 5.1889000e-10 /
CHEB / 1.3389000e-01 6.5931000e-10 4.5892000e-10 /
CHEB / 5.0206000e-02 5.4926000e-10 3.8233000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[OH]CHcH2+sC4H8O(+m)=C4H6O(717)+CH3CH[OH]CH2CH2(+m)     1.0E0 0.0
0.0   !NetReaction from PDepNetwork #68 (C8H15O2J(699))
      deltaHrxn(T=298K) = -1.9997127507831323 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9478000e+00 3.6733000e-10 2.5569000e-10 /
CHEB / 1.7084000e+01 6.9680000e-10 4.8503000e-10 /
CHEB / 3.3292000e-01 5.9888000e-10 4.1687000e-10 /
CHEB / 1.1932000e-01 4.7265000e-10 3.2900000e-10 /
CHEB / 4.0301000e-02 3.4629000e-10 2.4104000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
```

```
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

MEKenol+CH3C[OH]CHcH2(+m)=CH3CH[OH]CHCH3+C4H6O(717)(+m)     1.0E0 0.0
0.0   !NetReaction from PDepNetwork #138 (C8H15O2J(770))
      deltaHrxn(T=298K) = 2.779976811932684 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9275000e+00 3.1109000e-10 2.1654000e-10 /
CHEB / 1.7088000e+01 5.9712000e-10 4.1565000e-10 /
CHEB / 3.4289000e-01 5.2933000e-10 3.6846000e-10 /
CHEB / 1.3413000e-01 4.3620000e-10 3.0363000e-10 /
CHEB / 4.9644000e-02 3.3538000e-10 2.3345000e-10 /

sC4H8O+CH3C[OH]CHcH2(+m)=CH3CH[OH]CHCH3+C4H6O(717)(+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #138 (C8H15O2J(770))
      deltaHrxn(T=298K) = -4.6493711028735305 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7923000e+00 3.5384000e-10 2.4630000e-10 /
CHEB / 1.6992000e+01 6.7965000e-10 4.7309000e-10 /
CHEB / 3.5465000e-01 6.0381000e-10 4.2030000e-10 /
CHEB / 1.4313000e-01 4.9897000e-10 3.4732000e-10 /
CHEB / 6.0449000e-02 3.8462000e-10 2.6772000e-10 /

sC4H8O+CH3C[OH]CHcH2(+m)=MEKenol+CH3C[OH]CHcH2(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #138 (C8H15O2J(770))
      deltaHrxn(T=298K) = -7.4293479148062165 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9892000e+01 -1.9372000e-05 -1.3484000e-05 /
CHEB / 2.2399000e+01 1.8162000e-05 1.2642000e-05 /
CHEB / 1.7544000e+00 5.3365000e-06 3.7145000e-06 /
CHEB / 4.7169000e-01 -3.2650000e-06 -2.2726000e-06 /
CHEB / 1.2269000e-01 -1.5716000e-06 -1.0940000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     C2H5O-1           -7.2  70.51 14.71 17.83 20.61 23.05 26.99 29.97
      32.69 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH3C[O]CH2cH2     -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(1151)  -40.72      90.25 26.29 31.91 36.7  40.82 47.76 52.72
      57.44 null
!     nC3H7OH     -61.13      76.52 20.98 26.14 30.77 34.8  41.22 46.05
      51.6  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+CH2OH(+m)=CH3CO+C2H5O-1(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
2.9795891434437216 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1496000e+01 -1.3078000e+00 -6.1408000e-02 /
CHEB / 1.6144000e+00 1.0416000e+00 -3.9564000e-02 /
CHEB / 1.4711000e-01 4.2059000e-01 5.6951000e-02 /
CHEB / -2.4318000e-01 8.7676000e-03 5.8048000e-02 /
CHEB / -1.6198000e-01 -1.0617000e-01 1.2384000e-02 /

CH3C[O]CH2cH2+OH(+m)=CH3CO+C2H5O-1(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
10.918468984262237 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2572000e+01 -1.1598000e+00 -1.0564000e-01 /
CHEB / 1.1348000e+00 1.0257000e+00 6.5521000e-03 /
CHEB / 1.1988000e-01 3.0635000e-01 8.6556000e-02 /
CHEB / -1.5537000e-01 -4.7550000e-02 4.4718000e-02 /
CHEB / -1.1429000e-01 -1.0035000e-01 -6.7561000e-03 /

CH3C[O]CH2cH2+OH(+m)=CH2C[O]CH3+CH2OH(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
7.938879840818517 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0907000e+01 -1.1400000e+00 -1.0927000e-01 /
CHEB / 1.9266000e+00 1.0260000e+00 1.2000000e-02 /
CHEB / 3.1590000e-01 2.8924000e-01 8.9464000e-02 /
CHEB / -9.0445000e-02 -5.6534000e-02 4.1990000e-02 /
CHEB / -8.7576000e-02 -9.9500000e-02 -9.5304000e-03 /

sSPC(1151)+H(+m)=CH3CO+C2H5O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
17.757610414790275 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2554000e+01 -9.3371000e-01 -1.7577000e-01 /
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CHEB / 8.9393000e-02 8.6646000e-01 1.0353000e-01 /
CHEB / 9.7979000e-02 2.2021000e-01 8.5796000e-02 /
CHEB / -6.2821000e-02 -6.3767000e-02 2.1907000e-02 /
CHEB / -4.8103000e-02 -8.1450000e-02 -1.8330000e-02 /

sSPC(1151)+H(+m)=CH2C[O]CH3+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
14.778021271346555 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0951000e+01 -9.1904000e-01 -1.7642000e-01 /
CHEB / 8.2229000e-01 8.6483000e-01 1.0699000e-01 /
CHEB / 2.9754000e-01 2.0781000e-01 8.5950000e-02 /
CHEB / 3.2108000e-03 -6.8852000e-02 1.9221000e-02 /
CHEB / -2.2518000e-02 -8.0212000e-02 -1.9771000e-02 /

sSPC(1151)+H(+m)=CH3C[O]CH2cH2+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
6.839141430528036 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5712000e+00 -8.3670000e-01 -1.8221000e-01 /
CHEB / 2.0693000e+00 8.3569000e-01 1.2716000e-01 /
CHEB / 5.9156000e-01 1.4695000e-01 8.3717000e-02 /
CHEB / 8.3031000e-02 -8.3354000e-02 5.3734000e-03 /
CHEB / 8.4180000e-03 -6.9582000e-02 -2.4446000e-02 /

CH3CO+C2H5O-1(+m)=nC3H7OH+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
78.06228196749554 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1029000e+00 -6.5605000e-01 -2.1443000e-01 /
CHEB / 1.0425000e+01 6.1924000e-01 1.7531000e-01 /
CHEB / 4.9490000e-01 1.5466000e-01 6.8830000e-02 /
CHEB / 9.0930000e-02 -5.8727000e-02 -2.9929000e-04 /
CHEB / 1.2878000e-02 -6.0088000e-02 -2.1493000e-02 /

CH2C[O]CH3+CH2OH(+m)=nC3H7OH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
81.04187111093927 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5714000e-01 -6.4724000e-01 -2.1297000e-01 /
CHEB / 9.8921000e+00 6.1819000e-01 1.7650000e-01 /
CHEB / 5.7716000e-01 1.4688000e-01 6.7476000e-02 /
CHEB / 9.8574000e-02 -6.1589000e-02 -2.0591000e-03 /
CHEB / -1.3331000e-03 -5.9059000e-02 -2.1952000e-02 /

CH3C[O]CH2cH2+OH(+m)=nC3H7OH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
88.98075095175778 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8603000e+00 -6.0152000e-01 -2.0587000e-01 /
CHEB / 8.0324000e+00 6.0528000e-01 1.8123000e-01 /
CHEB / 8.1072000e-01 1.0891000e-01 6.0023000e-02 /
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CHEB / 1.7020000e-01 -7.0529000e-02 -9.8433000e-03 /
CHEB / 2.3950000e-02 -5.1730000e-02 -2.2855000e-02 /

sSPC(1151)+H(+m)=nC3H7OH+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
95.81989238228581 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8661000e+00 -5.4740000e-01 -1.9825000e-01 /
CHEB / 5.8274000e+00 5.7462000e-01 1.8414000e-01 /
CHEB / 1.0043000e+00 7.3778000e-02 5.1180000e-02 /
CHEB / 2.5482000e-01 -7.0999000e-02 -1.5968000e-02 /
CHEB / 7.7195000e-02 -4.2714000e-02 -2.1777000e-02 /

CH3CO+C2H5O-1(+m)=C4H6O(717)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
78.71227232324422 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7408000e+00 -1.4482000e+00 -4.3478000e-02 /
CHEB / 1.5682000e+00 9.2191000e-01 -5.0842000e-02 /
CHEB / 2.9173000e-01 5.1743000e-01 1.4198000e-02 /
CHEB / -1.9138000e-01 1.4833000e-01 4.4897000e-02 /
CHEB / -1.7169000e-01 -4.3834000e-02 3.1671000e-02 /

CH2C[O]CH3+CH2OH(+m)=C4H6O(717)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
81.69186146668795 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9115000e+00 -1.4251000e+00 -4.7503000e-02 /
CHEB / 1.5438000e+00 9.4370000e-01 -5.0655000e-02 /
CHEB / 2.8435000e-01 5.0375000e-01 2.1891000e-02 /
CHEB / -1.8862000e-01 1.2504000e-01 4.9182000e-02 /
CHEB / -1.7499000e-01 -5.5995000e-02 2.9762000e-02 /

CH3C[O]CH2cH2+OH(+m)=C4H6O(717)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #192 (C4H8O2(939)) deltaHrxn(T=298K) = -
89.63074130750647 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0340000e+01 -1.2702000e+00 -9.2111000e-02 /
CHEB / 1.6828000e+00 9.8449000e-01 -1.8693000e-02 /
CHEB / 1.9245000e-01 3.9656000e-01 6.5071000e-02 /
CHEB / -1.2105000e-01 2.9395000e-02 5.4412000e-02 /
CHEB / -1.1031000e-01 -8.2754000e-02 1.1565000e-02 /

sSPC(1151)+H(+m)=C4H6O(717)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
96.4698827380345 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9697000e+00 -1.0212000e+00 -1.7468000e-01 /
CHEB / 9.1114000e-01 8.5317000e-01 8.2557000e-02 /
CHEB / 1.8490000e-01 2.9301000e-01 8.1287000e-02 /
CHEB / -3.1740000e-02 -1.7388000e-02 3.7251000e-02 /
CHEB / -3.7327000e-02 -7.7157000e-02 -6.0904000e-03 /
```

```
nC3H7OH+CO(+m)=C4H6O(717)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #192 (C4H8O2(939))      deltaHrxn(T=298K) = -
0.6499903557486775 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3887000e+01 -7.1195000e-01 -2.2445000e-01 /
CHEB / 3.7912000e+01 6.1475000e-01 1.6537000e-01 /
CHEB / 5.7674000e-01 2.0321000e-01 7.5843000e-02 /
CHEB / 1.2065000e-01 -3.2513000e-02 1.2080000e-02 /
CHEB / 3.1060000e-02 -6.0835000e-02 -1.6037000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     C3H4O-enone       -15.03      68.27 16.5  19.56 22.34 24.77 28.73
      31.72 36.36 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[O]cHCH3+OH(+m)=CH3CO+C2H5O-2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
13.728431498127918 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1829000e+01 -9.4512000e-01 -1.6031000e-01 /
CHEB / 6.7449000e-01 9.2268000e-01 9.0883000e-02 /
CHEB / 6.1920000e-02 1.8652000e-01 8.9951000e-02 /
CHEB / -9.7672000e-02 -8.3241000e-02 2.0339000e-02 /
CHEB / -5.8903000e-02 -7.3457000e-02 -2.2096000e-02 /

CH3CO+C2H5O-2(+m)=C4H6O(717)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
73.0026386141389 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.0282000e+01 -1.3795000e+00 -4.9848000e-02 /
CHEB / 1.5771000e+00 9.9895000e-01 -4.6307000e-02 /
CHEB / 1.5597000e-01 4.9703000e-01 3.6675000e-02 /
CHEB / -1.5872000e-01 9.0127000e-02 6.0352000e-02 /
CHEB / -1.0265000e-01 -8.2805000e-02 3.0453000e-02 /

CH3C[O]cHCH3+OH(+m)=C4H6O(717)+H2O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
86.73107011226682 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0497000e+01 -1.0221000e+00 -1.6807000e-01 /
CHEB / 1.0069000e+00 9.0718000e-01 7.9157000e-02 /
CHEB / 2.0288000e-02 2.7933000e-01 8.8888000e-02 /
CHEB / -9.6003000e-02 -4.3491000e-02 4.3008000e-02 /
CHEB / -6.4230000e-02 -8.3068000e-02 -9.4295000e-03 /

CH3CO+C2H5O-2(+m)=CH3OH+C3H4O-enone(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
47.83185073228112 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9084000e+00 -1.2927000e+00 -5.9157000e-02 /
CHEB / 2.7881000e+00 1.0603000e+00 -3.6224000e-02 /
CHEB / 3.8481000e-01 4.1365000e-01 6.1559000e-02 /
CHEB / -8.5912000e-02 -3.5764000e-03 5.9542000e-02 /
CHEB / -3.9152000e-02 -1.1002000e-01 1.0270000e-02 /

CH3C[O]cHCH3+OH(+m)=CH3OH+C3H4O-enone(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
61.56028223040904 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8521000e+00 -9.7023000e-01 -1.6062000e-01 /
CHEB / 1.5828000e+00 9.2318000e-01 8.6581000e-02 /
CHEB / 2.8918000e-01 2.1368000e-01 8.9495000e-02 /
CHEB / -8.7817000e-03 -7.5075000e-02 2.6383000e-02 /
CHEB / -2.5140000e-02 -7.7609000e-02 -1.9484000e-02 /

CH3OH+C3H4O-enone(+m)=C4H6O(717)+H2O(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #221 (C4H8O2(940)) deltaHrxn(T=298K) = -
25.170787881857777 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0161000e+01 -1.4219000e+00 -4.2766000e-02 /
CHEB / 1.7980000e+01 9.6294000e-01 -4.7458000e-02 /
CHEB / 5.4630000e-01 5.3145000e-01 2.1865000e-02 /
CHEB / -1.2056000e-01 1.3843000e-01 5.4206000e-02 /
CHEB / -1.3434000e-01 -6.2761000e-02 3.7582000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3C[O]CH2cH2     -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     sSPC(1151)  -40.72      90.25 26.29 31.91 36.7  40.82 47.76 52.72
      57.44 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[O]CH2cH2+CH3CH[o]C2H3(+m)=sSPC(1151)+C4H7-24(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #375 (C8H14O2(772))
      deltaHrxn(T=298K) = -12.66876386822188 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4029000e+00 -1.4164000e+00 -2.9520000e-02 /
CHEB / 2.6303000e+00 9.9475000e-01 -3.0481000e-02 /
CHEB / 3.5719000e-01 5.8298000e-01 2.5711000e-02 /
CHEB / -4.1440000e-01 1.5855000e-01 5.4464000e-02 /
CHEB / -3.4282000e-01 -1.0322000e-01 3.2597000e-02 /

CH3C[O]CH2cH2+CH3CH[o]C2H3(+m)=C4H6O(717)+sC4H8O(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #375 (C8H14O2(772))
      deltaHrxn(T=298K) = -74.47228234612686 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0605000e+00 -1.4322000e+00 -2.3320000e-02 /
CHEB / 2.6596000e+00 9.8107000e-01 -2.4051000e-02 /
CHEB / 4.6944000e-01 6.0303000e-01 2.1235000e-02 /
CHEB / -3.3441000e-01 1.9256000e-01 4.5624000e-02 /
CHEB / -3.3544000e-01 -8.7931000e-02 2.7987000e-02 /

sSPC(1151)+C4H7-24(+m)=C4H6O(717)+sC4H8O(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #375 (C8H14O2(772))
      deltaHrxn(T=298K) = -61.80351847790499 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1358000e+00 -1.4598000e+00 -1.7340000e-02 /
CHEB / 3.6930000e+00 9.4997000e-01 -1.9291000e-02 /
```

```
CHEB / 6.2542000e-01 6.2081000e-01 1.2770000e-02 /
CHEB / -3.7480000e-01 2.3895000e-01 3.2574000e-02 /
CHEB / -3.9662000e-01 -5.4898000e-02 2.3199000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[O]cHCH3+CH3C[O]cHCH3(+m)=C4H6O(717)+MEKenol(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #466 (C8H14O2(897))
      deltaHrxn(T=298K) = -55.51425596199583 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3769000e+00 -1.4587000e+00 -3.3700000e-02 /
CHEB / 4.1397000e+00 9.3792000e-01 -4.1520000e-02 /
CHEB / 5.7408000e-01 5.8700000e-01 1.1758000e-02 /
CHEB / -3.2735000e-01 2.1041000e-01 4.6216000e-02 /
CHEB / -3.5145000e-01 -4.6451000e-02 4.0044000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[O]cHCH3+C4H6O(717)(+m)=C4H6O(717)+CH3C[OH]CHcH2(+m)    1.0E0 0.0
0.0   !NetReaction from PDepNetwork #637 (C8H13O2J(654))
      deltaHrxn(T=298K) = 0.19992958293743435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3948000e+00 -1.3129000e-03 -9.1220000e-04 /
CHEB / 1.7564000e+01 -1.2100000e-03 -8.3929000e-04 /
CHEB / 3.9260000e-01 -1.0935000e-03 -7.5846000e-04 /
CHEB / 1.3104000e-01 -1.0516000e-03 -7.2959000e-04 /
CHEB / 3.7017000e-02 -7.5023000e-04 -5.2024000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[o]C2H3+C4H7-22(+m)=C4H7-24+CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #775 (C8H14O(888))
      deltaHrxn(T=298K) = -44.28551653196809 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3268000e+01 -7.5247000e-01 -2.2784000e-01 /
CHEB / -4.9578000e-01 7.0937000e-01 1.7315000e-01 /
CHEB / 5.3454000e-02 1.9144000e-01 9.1585000e-02 /
CHEB / -9.1564000e-02 -6.0931000e-02 1.1150000e-02 /
CHEB / -8.6384000e-02 -7.8524000e-02 -2.7046000e-02 /

C4H7-24+CH3C[O]cHCH3(+m)=C4H6-13+MEKenol(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #775 (C8H14O(888))
      deltaHrxn(T=298K) = -42.695679820100395 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 4.9080000e+00 -1.3457000e+00 -4.5842000e-02 /
CHEB / 5.9354000e+00 1.0510000e+00 -3.6833000e-02 /
CHEB / 5.8214000e-01 5.0344000e-01 5.0791000e-02 /
CHEB / -1.6927000e-01 5.1519000e-02 6.9870000e-02 /
CHEB / -1.5700000e-01 -1.3408000e-01 2.2081000e-02 /

CH3CH[o]C2H3+C4H7-22(+m)=C4H6-13+MEKenol(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #775 (C8H14O(888))
      deltaHrxn(T=298K) = -86.98119635206848 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0784000e+00 -7.5118000e-01 -2.2298000e-01 /
CHEB / 1.4509000e+00 7.1705000e-01 1.7013000e-01 /
CHEB / 6.0075000e-01 1.8074000e-01 8.9315000e-02 /
CHEB / 8.8702000e-02 -6.5922000e-02 8.7305000e-03 /
CHEB / -2.3056000e-02 -7.6229000e-02 -2.7053000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[OH]CHCH3+CH3CH[o]C2H3(+m)=MEKenol+sC4H8O(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #906 (C8H16O2(782))
      deltaHrxn(T=298K) = -74.55251754575734 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2865000e+00 -1.4062000e+00 -3.4131000e-02 /
```

```
CHEB / 2.5985000e+00 1.0059000e+00 -3.4918000e-02 /
CHEB / 3.6605000e-01 5.7556000e-01 3.0510000e-02 /
CHEB / -3.3558000e-01 1.4042000e-01 6.3703000e-02 /
CHEB / -2.7518000e-01 -1.1573000e-01 3.7663000e-02 /

CH3CH[OH]CHCH3+CH3CH[o]C2H3(+m)=sC4H8O+sC4H8O(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #906 (C8H16O2(782))
      deltaHrxn(T=298K) = -67.12316963095112 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0976000e+00 -1.4024000e+00 -3.5626000e-02 /
CHEB / 3.2586000e+00 1.0091000e+00 -3.6475000e-02 /
CHEB / 5.2435000e-01 5.7061000e-01 3.1455000e-02 /
CHEB / -2.9109000e-01 1.3248000e-01 6.5486000e-02 /
CHEB / -2.5434000e-01 -1.1892000e-01 3.8507000e-02 /

sC4H8O+sC4H8O(+m)=MEKenol+sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #906 (C8H16O2(782))      deltaHrxn(T=298K) = -
7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4197000e+01 -1.4514000e+00 -2.0782000e-02 /
CHEB / 2.1293000e+01 9.5951000e-01 -2.2693000e-02 /
CHEB / 8.7392000e-01 6.1501000e-01 1.6485000e-02 /
CHEB / -3.0628000e-01 2.2336000e-01 4.0253000e-02 /
CHEB / -3.1825000e-01 -6.6429000e-02 2.7813000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:
```

```
CH3CH[OH]CHCH3+CH3C[O]cHCH3(+m)=MEKenol+MEKenol(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1017 (C8H16O2(907))
      deltaHrxn(T=298K) = -58.49416235686595 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0135000e+00 -1.4355000e+00 -2.2852000e-02 /
CHEB / 4.2764000e+00 9.7527000e-01 -2.4083000e-02 /
CHEB / 5.9187000e-01 5.9997000e-01 1.9198000e-02 /
CHEB / -3.4649000e-01 1.9415000e-01 4.2601000e-02 /
CHEB / -3.3531000e-01 -8.2008000e-02 2.6733000e-02 /

CH3CH[OH]CHCH3+CH3C[O]cHCH3(+m)=sC4H8O+MEKenol(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1017 (C8H16O2(907))
      deltaHrxn(T=298K) = -51.064814442059735 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3601000e+00 -1.4234000e+00 -2.6124000e-02 /
CHEB / 5.5915000e+00 9.8722000e-01 -2.6926000e-02 /
CHEB / 7.5699000e-01 5.8854000e-01 2.2817000e-02 /
CHEB / -2.9609000e-01 1.7202000e-01 4.8011000e-02 /
CHEB / -2.9622000e-01 -9.3880000e-02 2.8439000e-02 /

sC4H8O+MEKenol(+m)=MEKenol+MEKenol(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1017 (C8H16O2(907))     deltaHrxn(T=298K) = -
7.429347914806215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5704000e+01 -1.4428000e+00 -2.1246000e-02 /
CHEB / 2.2432000e+01 9.6740000e-01 -2.2812000e-02 /
CHEB / 9.8741000e-01 6.0529000e-01 1.7044000e-02 /
CHEB / -2.1412000e-01 2.0644000e-01 3.9503000e-02 /
CHEB / -2.8182000e-01 -7.4118000e-02 2.5831000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
```

```
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

CH3CH[OH]CH2CH2+CH3C[O]cHCH3(+m)=sC4H8O+MEKenol(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1138 (C8H16O2(905))
      deltaHrxn(T=298K) = -53.71447279415013 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4719000e+00 -1.4247000e+00 -2.6572000e-02 /
CHEB / 4.6130000e+00 9.8589000e-01 -2.7576000e-02 /
CHEB / 6.4043000e-01 5.8964000e-01 2.2871000e-02 /
CHEB / -3.4081000e-01 1.7410000e-01 4.8857000e-02 /
CHEB / -3.2522000e-01 -9.2843000e-02 2.9429000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3CO       -1.95 63.74 12.06 14.11 16.08 17.82 20.67 22.81 26.16
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH3C[O]cHCH3=sSPC(752)     3.7700000e+12      0.00000
0.0000000e+00
!     sSPC(752)=HO2+C4H6O(717)      4.3669559e+09      1.31333
2.9866667e+04

O2+CH3C[O]cHCH3(+m)=sSPC(752)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(752)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H/OneDeC          deltaHrxn(T=298K) = -
33.1765152908666 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2215000e+01 7.9713000e-01 -1.0149000e-01 /
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CHEB / -2.0447000e+00 1.0184000e+00 -2.0812000e-02 /
CHEB / -8.0399000e-01 3.0540000e-01 8.2182000e-02 /
CHEB / -3.0760000e-01 -3.1776000e-02 5.6189000e-02 /
CHEB / -1.1389000e-01 -6.7357000e-02 4.0507000e-03 /

sSPC(752)(+m)=HO2+C4H6O(717)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(752)) High-P Limit:
HO2_Elimination_from_PeroxyRadical estimate: (Average:) R2OO_2H_HDe
      deltaHrxn(T=298K) = 15.94839865155285 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8246000e-01 6.4793000e-01 -6.1476000e-02 /
CHEB / 8.6615000e+00 9.9247000e-01 -4.8944000e-02 /
CHEB / -7.0463000e-01 4.3136000e-01 4.5502000e-02 /
CHEB / -3.3080000e-01 5.2085000e-02 5.7395000e-02 /
CHEB / -1.1300000e-01 -6.2367000e-02 2.1126000e-02 /

O2+CH3C[O]cHCH3(+m)=HO2+C4H6O(717)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(752))     deltaHrxn(T=298K) = -
17.228116639313747 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1851000e+01 -9.9624000e-01 -1.2187000e-01 /
CHEB / 9.4909000e-01 1.0285000e+00 3.3098000e-02 /
CHEB / -4.9608000e-02 1.1986000e-01 1.0259000e-01 /
CHEB / -1.1786000e-01 -1.1197000e-01 1.9070000e-02 /
CHEB / -2.5768000e-02 -5.6158000e-02 -2.3362000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(752)+H(+m)=HO2+CH3C[O]cHCH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #63 (C4H8O3(354))  deltaHrxn(T=298K) = -
16.067985660482734 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4647000e+00 -1.4803000e-02 -1.0281000e-02 /
CHEB / 5.8090000e-01 1.8115000e-02 1.2579000e-02 /
CHEB / 4.1299000e-01 -9.5505000e-04 -6.6159000e-04 /
CHEB / 1.4288000e-01 -2.8039000e-03 -1.9437000e-03 /
CHEB / 3.5811000e-02 -5.8446000e-05 -4.3938000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3C[OH]cH  20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23 39.84
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

CH2OOH+CH3C[OH]cH(+m)=HO2+CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #82 (C4H8O3(829)) deltaHrxn(T=298K)
= -45.445115015767705 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1251000e+01 -5.3953000e-03 -3.7392000e-03 /
```

```
CHEB / -1.3747000e-01 5.5723000e-03 3.8593000e-03 /
CHEB / 1.4551000e-01 6.7342000e-04 4.6820000e-04 /
CHEB / 7.5036000e-02 -1.0240000e-03 -7.0811000e-04 /
CHEB / 2.7036000e-02 -3.4794000e-04 -2.4199000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2C[OH]CH2cH2    5.43  85.83 23.53 28.76 33.18 36.91 43.01 47.46
      54.07 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH2C[OH]CH2 -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26 40.88
      null
!     C2H3O-2           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!Here are the path reactions and their high-P limit kinetics:

CH2OOH+CH2C[OH]CH2(+m)=HO2+CH2C[OH]CH2cH2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #107 (C4H8O3(830))
      deltaHrxn(T=298K) = -6.439098465350254 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0574000e+00 -7.1621000e-02 -4.5630000e-02 /
CHEB / 1.8258000e+00 9.2058000e-02 5.7973000e-02 /
CHEB / 5.4539000e-01 -1.2489000e-02 -6.8938000e-03 /
CHEB / 9.2431000e-02 -1.1324000e-02 -7.4576000e-03 /
CHEB / -2.2169000e-03 5.5667000e-04 7.4148000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(116)+CH3C[O]cHCH3(+m)=sSPC(752)+CH3CH[OH]CHCH3(+m)     1.0E0 0.0
0.0   !NetReaction from PDepNetwork #141 (C8H16O4(427))
      deltaHrxn(T=298K) = 1.7200187330861283 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2856000e+00 -3.3629000e-01 -1.5407000e-01 /
CHEB / 4.5158000e+00 4.2053000e-01 1.8047000e-01 /
CHEB / 7.9158000e-01 -3.2389000e-02 4.4810000e-03 /
CHEB / 5.4898000e-02 -6.1812000e-02 -3.1060000e-02 /
CHEB / -4.3555000e-02 -5.1297000e-03 -8.7517000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
```

```
!Here are the path reactions and their high-P limit kinetics:

sSPC(332)+CH3C[O]cHCH3(+m)=CH3CH[OH]CH2CH2+sSPC(752)(+m)    1.0E0 0.0
0.0   !NetReaction from PDepNetwork #173 (C8H16O4(708))
      deltaHrxn(T=298K) = 1.4282060588044487E-4 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7781000e+00 -3.1770000e-01 -1.4882000e-01 /
CHEB / 4.6239000e+00 3.9952000e-01 1.7611000e-01 /
CHEB / 8.6239000e-01 -3.4131000e-02 1.6439000e-03 /
CHEB / 8.5374000e-02 -5.7979000e-02 -2.9935000e-02 /
CHEB / -3.1140000e-02 -3.6123000e-03 -7.4146000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(46)+CH3C[O]cHCH3(+m)=sSPC(752)+C4H7-24(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #215 (C8H14O3(489))
      deltaHrxn(T=298K) = -12.668620907906785 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3112000e+00 -2.2967000e-01 -1.2197000e-01 /
CHEB / 2.2646000e+00 2.8615000e-01 1.4628000e-01 /
CHEB / 5.4123000e-01 -2.0715000e-02 -2.2000000e-03 /
CHEB / 6.9794000e-02 -4.2537000e-02 -2.3575000e-02 /
CHEB / -2.6253000e-02 -3.4017000e-03 -4.7156000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+CH3C[O]cHCH3(+m)=C4H7-24+sSPC(752)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #289 (C8H14O3(584))
      deltaHrxn(T=298K) = -14.238447734511418 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0900000e+00 -2.0688000e-01 -1.1434000e-01 /
CHEB / 1.8081000e+00 2.5404000e-01 1.3598000e-01 /
CHEB / 5.3042000e-01 -1.2374000e-02 -1.6958000e-04 /
CHEB / 8.9849000e-02 -3.9778000e-02 -2.2464000e-02 /
CHEB / -2.0295000e-02 -5.1970000e-03 -5.1019000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1072)  -76.48      99.01 32.08 38.74 44.26 48.98 56.59 62.32
      67.82 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     sSPC(1013)  -47.63      104.06      35.2  42.15 48.1  52.8  60.33
      66.06 72.62 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
sSPC(1013)+O(+m)=sSPC(1072)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #381 (C4H9O4J(852))     deltaHrxn(T=298K) = -
79.0719642220627 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0882000e+01 -1.8656000e-08 -1.2986000e-08 /
CHEB / 1.6587000e+00 -2.6067000e-08 -1.8145000e-08 /
CHEB / 2.7909000e-01 -4.1503000e-09 -2.8889000e-09 /
CHEB / 9.1842000e-02 1.0874000e-08 7.5694000e-09 /
CHEB / 1.0835000e-02 1.3913000e-08 9.6847000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(332)+CH3CH[OH]CHCH3(+m)=sSPC(116)+CH3CH[OH]CH2CH2(+m)  1.0E0 0.0
0.0   !NetReaction from PDepNetwork #1 (C8H18O4(339)) deltaHrxn(T=298K)
= -1.719875912480262 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7412000e+00 -5.4420000e-01 -1.8436000e-01 /
CHEB / 4.1565000e+00 6.5715000e-01 1.9265000e-01 /
CHEB / 8.4685000e-01 -1.7720000e-02 3.9098000e-02 /
CHEB / 4.4902000e-02 -1.0070000e-01 -3.6986000e-02 /
CHEB / -3.5352000e-02 -2.1657000e-02 -2.2972000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1072)  -76.48      99.01 32.08 38.74 44.26 48.98 56.59 62.32
      67.82 null
!     sSPC(1151)  -40.72      90.25 26.29 31.91 36.7  40.82 47.76 52.72
      57.44 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3C[O]CH2cH2     -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     sSPC(1151)+OH=sSPC(1072)      2.0000000e+13      0.00000
0.0000000e+00
!     HO2+CH3C[O]CH2cH2=sSPC(1072)  1.4157154e+13      -0.15000
2.9166667e+02
!     CH2OOH+CH2C[O]CH3=sSPC(1072)  1.1500000e+13      0.00000
0.0000000e+00

sSPC(1151)+OH(+m)=sSPC(1072)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (sSPC(1072)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
45.075239989650434 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1932000e+01 7.0160000e-01 -4.5386000e-02 /
CHEB / -4.0177000e+00 1.0500000e+00 -1.6575000e-02 /
CHEB / -2.5240000e+00 4.3289000e-01 5.2596000e-02 /
CHEB / -1.5060000e+00 2.3849000e-02 3.9786000e-02 /
CHEB / -7.8586000e-01 -1.0773000e-01 -2.7430000e-04 /

HO2+CH3C[O]CH2cH2(+m)=sSPC(1072)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1072)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     C_rad/H2/Cs          deltaHrxn(T=298K) = -
69.02314083512016 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8679000e+00 4.6909000e+00 -5.4217000e-01 /
CHEB / -4.9937000e+00 5.2998000e-01 2.3735000e-01 /
CHEB / -2.9741000e+00 1.3935000e-01 1.0488000e-01 /
CHEB / -1.5939000e+00 -9.6908000e-02 6.4303000e-03 /
CHEB / -7.9729000e-01 -1.1981000e-01 -1.5257000e-02 /
```

```
HO2+CH3C[O]CH2cH2(+m)=sSPC(1151)+OH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1072))    deltaHrxn(T=298K) = -
23.947900845469725 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3050000e+01 -1.1055000e-01 -7.5380000e-02 /
CHEB / -3.5164000e-01 1.3633000e-01 9.1645000e-02 /
CHEB / -5.4837000e-02 -6.8437000e-03 -2.8801000e-03 /
CHEB / -4.2882000e-02 -2.2392000e-02 -1.4955000e-02 /
CHEB / -2.9261000e-02 -1.6622000e-03 -2.0648000e-03 /

CH2OOH+CH2C[O]CH3(+m)=sSPC(1072)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1072)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     C_rad/H2/CO           deltaHrxn(T=298K) = -
88.57099574215287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1148000e-01 7.4249000e+00 4.2708000e-01 /
CHEB / -4.6311000e+00 3.1213000e-01 -7.1166000e-02 /
CHEB / -3.0002000e+00 -2.4406000e-02 5.6482000e-03 /
CHEB / -1.5787000e+00 -1.1266000e-01 -1.0450000e-02 /
CHEB / -7.8141000e-01 -1.1235000e-01 -1.9180000e-02 /

CH2OOH+CH2C[O]CH3(+m)=sSPC(1151)+OH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (sSPC(1072))    deltaHrxn(T=298K) = -
43.49575575250244 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3171000e+01 -2.4630000e-04 -2.0937000e-04 /
CHEB / -1.3612000e-01 2.7875000e-04 2.3686000e-04 /
CHEB / -3.2894000e-02 4.4153000e-05 3.7527000e-05 /
CHEB / -2.4280000e-02 -9.2647000e-05 -7.8642000e-05 /
CHEB / -2.5525000e-02 -6.2225000e-06 -5.2747000e-06 /

CH2OOH+CH2C[O]CH3(+m)=HO2+CH3C[O]CH2cH2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2 (sSPC(1072))   deltaHrxn(T=298K)
= -19.54785490703271 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9248000e+00 -8.1408000e-03 -5.6730000e-03 /
CHEB / 1.0490000e+00 9.6100000e-03 6.6982000e-03 /
CHEB / 4.3861000e-01 -3.4709000e-05 -2.6376000e-05 /
CHEB / 1.0578000e-01 -1.5593000e-03 -1.0860000e-03 /
CHEB / 1.3950000e-04 -1.6445000e-04 -1.1420000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HOCHOOH     -25.83      77.47 18.14 20.12 21.93 23.68 26.4  28.62
      29.35 null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
```

```
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3121)+H(+m)=CH2O+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -2.899226756297318
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5390000e+00 -6.5482000e-06 -4.5580000e-06 /
CHEB / 3.7496000e+00 -8.3003000e-06 -5.7775000e-06 /
CHEB / 3.5887000e-02 -6.1251000e-06 -4.2634000e-06 /
CHEB / 5.5243000e-02 -4.9373000e-06 -3.4367000e-06 /
CHEB / 4.0471000e-02 -3.7241000e-06 -2.5922000e-06 /

CH2OOH+O(+m)=CH2O+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -100.06953456442872
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3096000e+01 -4.6698000e-06 -3.2505000e-06 /
CHEB / -2.2574000e-01 -5.0015000e-06 -3.4814000e-06 /
CHEB / -5.6636000e-02 -3.3457000e-06 -2.3288000e-06 /
CHEB / -3.8796000e-02 -2.6780000e-06 -1.8641000e-06 /
CHEB / -2.4142000e-02 -1.9868000e-06 -1.3830000e-06 /

CH2OOH+O(+m)=sSPC(3121)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -97.17030780813141
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6615000e+00 -4.6142000e-06 -3.2118000e-06 /
CHEB / -9.9345000e-01 -4.8962000e-06 -3.4081000e-06 /
CHEB / -2.4036000e-01 -3.2545000e-06 -2.2654000e-06 /
CHEB / -9.9231000e-02 -2.6040000e-06 -1.8126000e-06 /
CHEB / -4.6975000e-02 -1.9304000e-06 -1.3437000e-06 /

CH2O+HO2(+m)=HOCHOOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -0.31016595502352473
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.7245000e+00 -6.3810000e-06 -4.4416000e-06 /
CHEB / 1.4082000e+01 -7.9737000e-06 -5.5502000e-06 /
CHEB / 4.7226000e-01 -5.8215000e-06 -4.0522000e-06 /
CHEB / 1.6612000e-01 -4.6696000e-06 -3.2503000e-06 /
CHEB / 6.6075000e-02 -3.5018000e-06 -2.4375000e-06 /
```

```
sSPC(3121)+H(+m)=HOCHOOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -3.2093927113208416
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2944000e+00 -6.3101000e-06 -4.3923000e-06 /
CHEB / 1.2886000e+01 -7.8356000e-06 -5.4541000e-06 /
CHEB / 5.7614000e-01 -5.6937000e-06 -3.9632000e-06 /
CHEB / 2.4190000e-01 -4.5575000e-06 -3.1723000e-06 /
CHEB / 1.0953000e-01 -3.4094000e-06 -2.3731000e-06 /

CH2OOH+O(+m)=HOCHOOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (CH3O3J(424))  deltaHrxn(T=298K) = -100.37970051945224
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6044000e+00 -4.4851000e-06 -3.1219000e-06 /
CHEB / 1.5665000e+00 -4.6529000e-06 -3.2387000e-06 /
CHEB / 4.7614000e-01 -3.0456000e-06 -2.1199000e-06 /
CHEB / 1.5998000e-01 -2.4363000e-06 -1.6958000e-06 /
CHEB / 5.6522000e-02 -1.8037000e-06 -1.2555000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+HO2(+m)=nSPC(801)+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C3H6O3JJ(464)) deltaHrxn(T=298K) =
1.5894264346048814 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6459000e+00 -3.5308000e-08 -2.4577000e-08 /
CHEB / 6.3154000e+00 -2.0277000e-08 -1.4114000e-08 /
CHEB / -8.0982000e-01 4.2639000e-08 2.9680000e-08 /
CHEB / -1.1587000e-01 3.9711000e-08 2.7642000e-08 /
CHEB / 1.0877000e-02 1.9908000e-09 1.3858000e-09 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     CH2OOH+CH3CO=sSPC(1474) 1.4157154e+13      -0.15000
2.9166667e+02
!     CH2C[O]CH3+HO2=sSPC(1474)     1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(3683)+H=sSPC(1474) 5.0000000e+13      0.00000
0.0000000e+00
!     sSPC(1590)+OH=sSPC(1474)      2.0000000e+13      0.00000
0.0000000e+00
!     sSPC(1356)+H=sSPC(1474) 1.4157154e+13      -0.15000
2.9166667e+02

CH2OOH+CH3CO(+m)=sSPC(1474)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     CO_rad/NonDe          deltaHrxn(T=298K) = -
81.18113040811039 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0538000e+00 1.9921000e+00 -5.4573000e-03 /
CHEB / -9.4164000e-01 7.1331000e-03 4.9325000e-03 /
CHEB / -4.3621000e-01 2.0801000e-03 1.4379000e-03 /
CHEB / -3.2939000e-02 -1.2166000e-03 -8.3751000e-04 /
CHEB / 6.4213000e-02 -7.7230000e-04 -5.3372000e-04 /

CH2C[O]CH3+HO2(+m)=sSPC(1474)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474)) High-P Limit: R_Recombination estimate:
```

```
(Average:) C_rad/H2/CO     O_rad/NonDe          deltaHrxn(T=298K) = -
65.97289352829706 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0234000e+01 1.9144000e+00 -5.5087000e-02 /
CHEB / -1.6112000e+00 8.3603000e-02 5.3485000e-02 /
CHEB / -6.3315000e-01 1.8211000e-02 1.1677000e-02 /
CHEB / -1.2777000e-01 -1.3022000e-02 -7.9079000e-03 /
CHEB / 1.8821000e-02 -7.2036000e-03 -4.6036000e-03 /

CH2OOH+CH3CO(+m)=CH2C[O]CH3+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -15.208236879813326
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2525000e+00 -5.9713000e-03 -4.1344000e-03 /
CHEB / 9.3360000e-01 6.6339000e-03 4.5905000e-03 /
CHEB / 3.7756000e-01 4.3436000e-04 3.0260000e-04 /
CHEB / 1.2251000e-01 -1.2156000e-03 -8.3950000e-04 /
CHEB / 3.1080000e-02 -2.5152000e-04 -1.7556000e-04 /

tSPC(3683)+H(+m)=sSPC(1474)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/CO     H_rad          deltaHrxn(T=298K) = -
96.27915303203716 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9867000e+00 1.9986000e+00 -9.7341000e-04 /
CHEB / -1.0602000e+00 1.1207000e-03 7.7925000e-04 /
CHEB / -2.9672000e-01 4.0272000e-04 2.8000000e-04 /
CHEB / 4.5717000e-02 -1.8626000e-04 -1.2941000e-04 /
CHEB / 9.6680000e-02 -1.5121000e-04 -1.0513000e-04 /

tSPC(3683)+H(+m)=CH2OOH+CH3CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -15.098022623926767
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4499000e+00 -1.0719000e-03 -7.4553000e-04 /
CHEB / 1.5359000e+00 1.0928000e-03 7.5994000e-04 /
CHEB / 7.3514000e-01 1.4877000e-04 1.0352000e-04 /
CHEB / 2.6722000e-01 -2.0094000e-04 -1.3968000e-04 /
CHEB / 8.4560000e-02 -7.0784000e-05 -4.9262000e-05 /

tSPC(3683)+H(+m)=CH2C[O]CH3+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -30.30625950374009
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1454000e+01 -1.1992000e-03 -8.3402000e-04 /
CHEB / 1.0901000e-01 1.1442000e-03 7.9560000e-04 /
CHEB / 2.9250000e-01 2.5250000e-04 1.7561000e-04 /
CHEB / 1.5528000e-01 -2.1410000e-04 -1.4880000e-04 /
CHEB / 5.6595000e-02 -1.0561000e-04 -7.3461000e-05 /

sSPC(1590)+OH(+m)=sSPC(1474)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474)) High-P Limit: R_Recombination estimate:
```

```
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
45.075239987272305 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2834000e+01 7.2016000e-01 -7.2005000e-02 /
CHEB / -2.2126000e+00 9.6515000e-01 -1.3846000e-02 /
CHEB / -9.7012000e-01 3.5899000e-01 4.9926000e-02 /
CHEB / -3.6898000e-01 3.0980000e-02 3.2079000e-02 /
CHEB / -7.8983000e-02 -4.9446000e-02 3.3585000e-03 /

CH2OOH+CH3CO(+m)=sSPC(1590)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -36.10589042083809
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2706000e+01 -7.0390000e-03 -4.8716000e-03 /
CHEB / -1.3911000e-02 7.1171000e-03 4.9229000e-03 /
CHEB / -8.2797000e-03 1.3413000e-03 9.2851000e-04 /
CHEB / 2.5672000e-02 -1.3448000e-03 -9.2718000e-04 /
CHEB / 1.3358000e-02 -5.6100000e-04 -3.8880000e-04 /

CH2C[O]CH3+HO2(+m)=sSPC(1590)+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #25 (sSPC(1474))   deltaHrxn(T=298K) = -
20.89765354102476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2975000e+01 -7.0940000e-02 -4.5862000e-02 /
CHEB / -2.6560000e-01 8.0082000e-02 5.1476000e-02 /
CHEB / -3.1904000e-02 4.8072000e-03 3.3104000e-03 /
CHEB / -1.0439000e-02 -1.4203000e-02 -8.8806000e-03 /
CHEB / -1.3314000e-02 -3.2932000e-03 -2.2855000e-03 /

tSPC(3683)+H(+m)=sSPC(1590)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -51.20391304476485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4255000e+01 -1.2966000e-03 -9.0171000e-04 /
CHEB / -3.8566000e-01 1.1508000e-03 8.0018000e-04 /
CHEB / 1.7922000e-02 3.3567000e-04 2.3341000e-04 /
CHEB / 6.4010000e-02 -2.0465000e-04 -1.4221000e-04 /
CHEB / 3.2993000e-02 -1.3149000e-04 -9.1441000e-05 /

sSPC(1356)+H(+m)=sSPC(1474)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
85.09098359516648 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4665000e+00 1.9955000e+00 -3.1299000e-03 /
CHEB / -1.3388000e+00 3.9520000e-03 2.7408000e-03 /
CHEB / -3.9186000e-01 1.2341000e-03 8.5571000e-04 /
CHEB / -8.2371000e-04 -6.6728000e-04 -4.6157000e-04 /
CHEB / 8.0541000e-02 -4.5576000e-04 -3.1596000e-04 /
```

```
sSPC(1356)+H(+m)=CH2OOH+CH3CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -3.9098531870560906
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4806000e+00 -2.7229000e-03 -1.8906000e-03 /
CHEB / 2.2893000e+00 3.1126000e-03 2.1604000e-03 /
CHEB / 8.0421000e-01 5.2370000e-07 1.1774000e-06 /
CHEB / 2.2941000e-01 -4.7611000e-04 -3.3035000e-04 /
CHEB / 6.9675000e-02 -8.3620000e-05 -5.8437000e-05 /

sSPC(1356)+H(+m)=CH2C[O]CH3+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -19.118090066869414
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0089000e+01 -3.5909000e-03 -2.4921000e-03 /
CHEB / 2.8542000e-01 3.8155000e-03 2.6470000e-03 /
CHEB / 3.5016000e-01 4.4715000e-04 3.1078000e-04 /
CHEB / 1.4245000e-01 -7.1823000e-04 -4.9759000e-04 /
CHEB / 4.5830000e-02 -2.1104000e-04 -1.4684000e-04 /

sSPC(1356)+H(+m)=sSPC(1590)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #25 (sSPC(1474))  deltaHrxn(T=298K) = -40.01574360789417
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3317000e+01 -4.0810000e-03 -2.8316000e-03 /
CHEB / -4.9521000e-01 3.9806000e-03 2.7610000e-03 /
CHEB / -1.0243000e-03 8.8004000e-04 6.1063000e-04 /
CHEB / 4.4848000e-02 -7.4061000e-04 -5.1269000e-04 /
CHEB / 2.5659000e-02 -3.5661000e-04 -2.4754000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     C2H5OH            -56.2 67.1  15.48 19.19 22.52 25.45 30.15 33.71
      37.35 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+OH(+m)=CH2OH+CH3CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -12.278497868037903
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2314000e+01 -8.4171000e-01 -1.8685000e-01 /
CHEB / 3.0387000e-01 8.1355000e-01 1.3069000e-01 /
CHEB / 5.7984000e-02 1.6552000e-01 7.7438000e-02 /
CHEB / -6.0857000e-02 -7.0697000e-02 1.2423000e-02 /
CHEB / -3.7594000e-02 -5.8408000e-02 -1.9367000e-02 /

sSPC(1590)+H(+m)=CH2OH+CH3CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -22.167886603010906
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3075000e+01 -3.8111000e-01 -1.7867000e-01 /
CHEB / -3.6966000e-01 3.7440000e-01 1.6734000e-01 /
CHEB / 3.7292000e-02 7.8859000e-02 4.1780000e-02 /
CHEB / 1.4334000e-02 -4.5247000e-02 -1.3807000e-02 /
CHEB / 1.4564000e-02 -2.8921000e-02 -1.4343000e-02 /

sSPC(1590)+H(+m)=CH2C[O]CH3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -9.889388734973005
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4543000e+00 -3.4109000e-01 -1.6315000e-01 /
CHEB / 7.7296000e-01 3.6412000e-01 1.6563000e-01 /
CHEB / 4.0191000e-01 3.9232000e-02 2.6544000e-02 /
CHEB / 1.1319000e-01 -4.8638000e-02 -1.7970000e-02 /
CHEB / 5.0552000e-02 -1.9192000e-02 -1.1942000e-02 /

CH2OH+CH3CO(+m)=C2H5OH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -76.7422635580607
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.1368000e-01 -2.5130000e-01 -1.3632000e-01 /
CHEB / 1.0371000e+01 2.4570000e-01 1.3020000e-01 /
CHEB / 3.8713000e-01 5.5873000e-02 3.1400000e-02 /
CHEB / 1.4344000e-01 -3.2725000e-02 -1.4026000e-02 /
CHEB / 6.0448000e-02 -2.0152000e-02 -1.1022000e-02 /

CH2C[O]CH3+OH(+m)=C2H5OH+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -89.0207614260986
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3292000e+00 -2.2940000e-01 -1.2560000e-01 /
CHEB / 7.0084000e+00 2.4146000e-01 1.2888000e-01 /
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CHEB / 6.4321000e-01 3.2905000e-02 2.0375000e-02 /
CHEB / 2.0280000e-01 -3.5612000e-02 -1.6458000e-02 /
CHEB / 6.8072000e-02 -1.4102000e-02 -8.7341000e-03 /

sSPC(1590)+H(+m)=C2H5OH+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -98.9101501610716
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0257000e+00 -1.8902000e-01 -1.0617000e-01 /
CHEB / 4.2316000e+00 2.1568000e-01 1.1769000e-01 /
CHEB / 9.1880000e-01 3.8553000e-03 6.1562000e-03 /
CHEB / 2.7253000e-01 -2.7271000e-02 -1.4161000e-02 /
CHEB / 1.1474000e-01 -7.2725000e-03 -5.6083000e-03 /

CH2OH+CH3CO(+m)=CH2CO+CH3OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -53.464484058528136
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9911000e+00 -1.3260000e+00 -5.7562000e-02 /
CHEB / 1.8088000e+00 1.0175000e+00 -3.7126000e-02 /
CHEB / 3.1829000e-01 4.2495000e-01 5.1506000e-02 /
CHEB / -8.5437000e-02 3.7060000e-02 5.1027000e-02 /
CHEB / -5.4396000e-02 -8.0581000e-02 1.1820000e-02 /

CH2C[O]CH3+OH(+m)=CH2CO+CH3OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -65.74298192656605
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4351000e+00 -8.9047000e-01 -1.8903000e-01 /
CHEB / 1.1055000e+00 8.1181000e-01 1.2238000e-01 /
CHEB / 2.2505000e-01 2.1367000e-01 7.8264000e-02 /
CHEB / 8.2840000e-03 -5.2622000e-02 2.1201000e-02 /
CHEB / -1.3727000e-02 -6.3578000e-02 -1.4354000e-02 /

sSPC(1590)+H(+m)=CH2CO+CH3OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -75.63237066153904
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9446000e+00 -3.9670000e-01 -1.8487000e-01 /
CHEB / 6.0892000e-01 3.7392000e-01 1.6619000e-01 /
CHEB / 2.3279000e-01 9.5483000e-02 4.8033000e-02 /
CHEB / 8.3937000e-02 -3.9513000e-02 -1.0484000e-02 /
CHEB / 4.2599000e-02 -3.1870000e-02 -1.4611000e-02 /

CH2CO+CH3OH(+m)=C2H5OH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #36 (C3H6O2(496)) deltaHrxn(T=298K) = -23.277779499532556
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4012000e+01 -2.6048000e-01 -1.4085000e-01 /
CHEB / 2.9615000e+01 2.4541000e-01 1.2971000e-01 /
CHEB / 5.8564000e-01 6.5881000e-02 3.6160000e-02 /
CHEB / 1.9210000e-01 -2.9361000e-02 -1.1972000e-02 /
```

```
CHEB / 6.8615000e-02 -2.2143000e-02 -1.1609000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+sSPC(116)(+m)=sSPC(1356)+CH3CH[OH]CHCH3(+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #49 (C7H14O4(492))
      deltaHrxn(T=298K) = 4.770123139472815 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4395000e+00 -4.1824000e-01 -1.7027000e-01 /
CHEB / 4.6940000e+00 5.1779000e-01 1.9232000e-01 /
CHEB / 6.6739000e-01 -3.3490000e-02 1.5145000e-02 /
CHEB / 3.4230000e-02 -7.5686000e-02 -3.4348000e-02 /
CHEB / -3.8913000e-02 -9.0704000e-03 -1.3115000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C3H6             4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+sSPC(332)(+m)=sSPC(1356)+CH3CH[OH]CH2CH2(+m)     1.0E0 0.0
0.0   !NetReaction from PDepNetwork #64 (C7H14O4(493))
      deltaHrxn(T=298K) = 3.0502472269925605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8116000e+00 -3.0121000e-01 -1.4440000e-01 /
CHEB / 4.0225000e+00 3.7568000e-01 1.7035000e-01 /
CHEB / 7.5440000e-01 -2.8168000e-02 1.6670000e-03 /
CHEB / 8.9474000e-02 -5.4939000e-02 -2.8134000e-02 /
CHEB / -2.1637000e-02 -4.3298000e-03 -7.1652000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+C4H7-24(+m)=CH3CH[o]C2H3+sSPC(1590)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #87 (C7H12O3(813))
      deltaHrxn(T=298K) = -20.50783830914425 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2124000e+01 -6.7909000e-01 -2.0481000e-01 /
CHEB / 5.1896000e-01 6.8593000e-01 1.5389000e-01 /
CHEB / -2.5220000e-02 5.8313000e-02 5.6689000e-02 /
CHEB / -8.7350000e-02 -8.7553000e-02 -1.3082000e-02 /
CHEB / -3.7101000e-02 -3.1345000e-02 -1.8991000e-02 /

sSPC(46)+CH2C[O]CH3(+m)=CH3CH[o]C2H3+sSPC(1590)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #87 (C7H12O3(813))
      deltaHrxn(T=298K) = -30.126354810664356 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2635000e+01 -4.1389000e-01 -1.8632000e-01 /
CHEB / 4.8417000e-02 4.1230000e-01 1.6527000e-01 /
CHEB / -2.6476000e-02 3.4150000e-02 2.7550000e-02 /
CHEB / -4.2962000e-02 -5.9588000e-02 -2.0520000e-02 /
CHEB / -2.3955000e-02 -1.6589000e-02 -1.1484000e-02 /

sSPC(46)+CH2C[O]CH3(+m)=sSPC(1356)+C4H7-24(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #87 (C7H12O3(813))
      deltaHrxn(T=298K) = -9.618516501520105 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4129000e+00 -3.1876000e-01 -1.5518000e-01 /
CHEB / 2.2817000e+00 3.5092000e-01 1.5670000e-01 /
CHEB / 5.3642000e-01 -8.6271000e-03 7.5520000e-03 /
CHEB / 7.0055000e-02 -5.3677000e-02 -2.4776000e-02 /
CHEB / -1.8036000e-02 -4.8376000e-03 -6.0659000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
```

```
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+CH2C[O]CH3(+m)=sSPC(1356)+C4H7-24(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #146 (C7H12O3(910))
      deltaHrxn(T=298K) = -11.18834332812473 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1182000e+00 -2.7851000e-01 -1.4014000e-01 /
CHEB / 1.8933000e+00 3.3817000e-01 1.6242000e-01 /
CHEB / 5.2590000e-01 -1.2276000e-02 5.1720000e-03 /
CHEB / 8.5066000e-02 -5.1633000e-02 -2.6324000e-02 /
CHEB / -1.1017000e-02 -8.9286000e-03 -8.4405000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1697)  3.82  64.41 12.08 14.18 16.24 18.05 20.9  23.01 26.26
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3O              4.87  54.42 9.87  11.64 13.32 14.81 17.21 19.04
      21.89
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH3=sSPC(1697)       2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+H=sSPC(1697)  5.0000000e+13      0.00000
0.0000000e+00
!     sSPC(1697)=CH2OOH       4.2390000e+09      1.45000
4.2270000e+04
```

```
!     CH2O+OH=CH2OOH          2.3501400e+11      0.30815
4.9629937e+03
!     nSPC(102)+H=CH2OOH      1.4157154e+13      -0.15000
2.9166667e+02
!     CH3O+O=sSPC(1697)       1.0000000e+13      0.00000
0.0000000e+00

CH2OOH(+m)=sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697))   deltaHrxn(T=298K) = -11.188401432299555
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8917000e+01 6.0652000e+00 2.9259000e-01 /
CHEB / 1.9120000e+01 -6.3481000e-01 1.8927000e-01 /
CHEB / -6.7809000e-01 -2.5777000e-01 6.9777000e-02 /
CHEB / -4.9456000e-01 7.3387000e-02 -3.9890000e-02 /
CHEB / -3.1673000e-01 1.7114000e-01 -6.9373000e-02 /

O2+CH3(+m)=sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697)) High-P Limit: R_Recombination exact:
O2_birad     C_methyl         deltaHrxn(T=298K) = -32.10610656861221
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0814000e+01 1.6938000e+00 -1.6327000e-01 /
CHEB / -1.9833000e+00 1.9774000e-01 1.0635000e-01 /
CHEB / -9.1792000e-01 7.6451000e-02 4.1304000e-02 /
CHEB / -4.4266000e-01 1.1988000e-02 6.5963000e-03 /
CHEB / -2.0118000e-01 -5.5493000e-03 -3.0919000e-03 /

O2+CH3(+m)=CH2OOH(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -20.917705136312655 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6113000e+01 1.9950000e+00 -4.2055000e-03 /
CHEB / 1.2645000e+01 3.4236000e-03 2.8110000e-03 /
CHEB / -3.3158000e-01 1.4307000e-03 1.1646000e-03 /
CHEB / -2.0777000e-01 1.6472000e-04 1.2291000e-04 /
CHEB / -1.0441000e-01 -1.4483000e-04 -1.2714000e-04 /

nSPC(102)+H(+m)=sSPC(1697)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     H_rad           deltaHrxn(T=298K) = -
99.37907311534353 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5013000e+01 4.8725000e+00 1.7581000e+00 /
CHEB / -1.1149000e+00 9.2004000e-01 -2.0403000e-01 /
CHEB / -4.0836000e-01 3.9346000e-01 -2.2501000e-01 /
CHEB / -3.2455000e-01 -6.2755000e-02 -2.0289000e-01 /
CHEB / -2.7262000e-01 -2.5631000e-01 -1.5373000e-01 /

nSPC(102)+H(+m)=CH2OOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
88.19067168304397 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -2.8975000e+01 2.0224000e+00 1.6000000e-02 /
CHEB / 8.6433000e+00 7.8534000e-03 5.8164000e-03 /
CHEB / -4.4548000e-01 2.9518000e-03 2.2246000e-03 /
CHEB / -2.7861000e-01 -1.0671000e-03 -7.4265000e-04 /
CHEB / -1.4376000e-01 -2.7849000e-03 -2.0290000e-03 /

nSPC(102)+H(+m)=O2+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697))   deltaHrxn(T=298K) = -67.27296654673131
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4289000e+01 2.6875000e-06 1.8708000e-06 /
CHEB / -7.8464000e-01 6.6492000e-07 4.6286000e-07 /
CHEB / -1.4241000e-01 -1.1546000e-06 -8.0376000e-07 /
CHEB / -5.9974000e-02 -1.1615000e-06 -8.0854000e-07 /
CHEB / -3.3652000e-02 -6.0223000e-07 -4.1921000e-07 /

sSPC(1697)(+m)=CH2O+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697))   deltaHrxn(T=298K) = -21.34837575836841
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0014000e+01 4.0902000e+00 3.0834000e-01 /
CHEB / 1.3735000e+01 -6.0258000e-01 2.1076000e-01 /
CHEB / -6.4933000e-01 -2.4559000e-01 7.8978000e-02 /
CHEB / -4.9877000e-01 7.7252000e-02 -3.6908000e-02 /
CHEB / -3.2674000e-01 1.7301000e-01 -6.8526000e-02 /

CH2OOH(+m)=CH2O+OH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -32.53677719066796 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7323000e+00 2.0000000e+00 -6.8628000e-08 /
CHEB / 1.9741000e+00 -1.9268000e-07 -1.3412000e-07 /
CHEB / -9.0507000e-01 -1.7957000e-07 -1.2500000e-07 /
CHEB / -4.0454000e-01 -1.5902000e-07 -1.1069000e-07 /
CHEB / -1.6656000e-01 -1.3264000e-07 -9.2327000e-08 /

!O2+CH3(+m)=CH2O+OH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -53.454482326980624 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 7.9619000e+00 -3.8296000e-03 -3.2044000e-03 /
!CHEB / 4.1702000e+00 4.0435000e-03 3.3719000e-03 /
!CHEB / 1.8822000e-01 6.1695000e-04 5.1730000e-04 /
!CHEB / 6.4399000e-02 -5.7037000e-04 -4.7253000e-04 /
!CHEB / 9.0910000e-03 -3.3058000e-04 -2.7403000e-04 /

nSPC(102)+H(+m)=CH2O+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697))   deltaHrxn(T=298K) = -120.72744887371194
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3420000e+01 -1.9106000e-05 -1.3301000e-05 /
CHEB / 2.2671000e-01 1.4643000e-05 1.0194000e-05 /
CHEB / 1.4069000e-01 5.9018000e-06 4.1085000e-06 /
```

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CHEB / 5.5835000e-02 7.7667000e-07 5.4057000e-07 /
CHEB / 1.3007000e-02 -1.0840000e-06 -7.5470000e-07 /

CH3O+O(+m)=sSPC(1697)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/NonDe     Oa       deltaHrxn(T=298K) = -
60.68347818461715 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3181000e-01 5.9363000e+00 1.1313000e+00 /
CHEB / -7.8261000e-01 -9.7504000e-01 -3.5792000e-01 /
CHEB / -3.7691000e-01 -6.4799000e-01 -1.3171000e-01 /
CHEB / -3.3862000e-01 -2.9738000e-01 7.7370000e-02 /
CHEB / -2.9527000e-01 -9.4690000e-02 1.5546000e-01 /

CH3O+O(+m)=CH2OOH(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -49.495076752317594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8150000e+01 2.1041000e+00 7.5602000e-02 /
CHEB / 9.0472000e+00 -8.9118000e-04 -1.1970000e-03 /
CHEB / -3.7737000e-01 -5.8483000e-03 -4.5118000e-03 /
CHEB / -2.6110000e-01 -5.4437000e-03 -3.8942000e-03 /
CHEB / -1.3573000e-01 -4.2995000e-03 -2.9676000e-03 /

CH3O+O(+m)=O2+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -28.57737161600494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3293000e+01 1.3730000e-05 9.5624000e-06 /
CHEB / -4.5034000e-01 9.8767000e-06 6.8795000e-06 /
CHEB / -1.1554000e-01 -5.0808000e-06 -3.5421000e-06 /
CHEB / -6.7690000e-02 -7.9215000e-06 -5.5187000e-06 /
CHEB / -4.4184000e-02 -5.1297000e-06 -3.5718000e-06 /

nSPC(102)+H(+m)=CH3O+O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (sSPC(1697))   deltaHrxn(T=298K) = -38.695594930726394
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2548000e+01 -9.4779000e-05 -6.5977000e-05 /
CHEB / -2.8445000e-01 7.6481000e-05 5.3240000e-05 /
CHEB / 7.8478000e-02 2.6320000e-05 1.8321000e-05 /
CHEB / 3.6757000e-02 -2.8581000e-07 -1.9931000e-07 /
CHEB / 4.0964000e-03 -5.2887000e-06 -3.6816000e-06 /

CH3O+O(+m)=CH2O+OH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (sSPC(1697))   deltaHrxn(T=298K) = -82.03185394298556 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1826000e+01 -7.7773000e-04 -5.4236000e-04 /
CHEB / 8.1093000e-01 6.9060000e-04 4.8174000e-04 /
CHEB / 2.8425000e-01 1.9562000e-04 1.3633000e-04 /
CHEB / 7.9077000e-02 -3.7604000e-05 -2.6313000e-05 /
CHEB / 7.8509000e-03 -5.6948000e-05 -3.9722000e-05 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1735)  -31.8 64.6  15.3  17.87 20.17 22.29 25.5  28.18 31.81
      null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!Here are the path reactions and their high-P limit kinetics:
!     CH2OOH+H=sSPC(1735)     5.0000000e+13      0.00000
0.0000000e+00
!     CH3+HO2=sSPC(1735)      1.2100000e+13      0.00000
0.0000000e+00
!     CH3O+OH=sSPC(1735)      2.0000000e+13      0.00000
0.0000000e+00
!     sSPC(1697)+H=sSPC(1735) 1.4157154e+13      -0.15000
2.9166667e+02

CH2OOH+H(+m)=sSPC(1735)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     H_rad           deltaHrxn(T=298K) = -
95.79962922631896 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7854000e+00 2.0000000e+00 -6.0732000e-06 /
CHEB / -5.2330000e-01 2.9511000e-06 2.0542000e-06 /
CHEB / -2.3745000e-01 3.7307000e-06 2.5969000e-06 /
CHEB / -4.0978000e-02 9.6603000e-07 6.7243000e-07 /
CHEB / 2.3773000e-02 -3.8704000e-07 -2.6941000e-07 /

CH3+HO2(+m)=sSPC(1735)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735)) High-P Limit: R_Recombination exact:
O_rad/NonDe     C_methyl      deltaHrxn(T=298K) = -67.03290138701146
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7942000e+00 1.9999000e+00 -8.0785000e-05 /
CHEB / -4.9267000e-01 5.4716000e-05 3.8084000e-05 /
CHEB / -3.9610000e-01 5.4224000e-05 3.7740000e-05 /
CHEB / -1.2865000e-01 1.0443000e-05 7.2685000e-06 /
CHEB / -2.0158000e-02 -7.5447000e-06 -5.2508000e-06 /
```

```
CH2OOH+H(+m)=CH3+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -28.766727839307503
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2202000e+01 -8.1537000e-06 -5.6755000e-06 /
CHEB / 7.1413000e-02 3.5919000e-06 2.5002000e-06 /
CHEB / 2.1188000e-01 3.6763000e-06 2.5590000e-06 /
CHEB / 1.4694000e-01 6.8999000e-07 4.8028000e-07 /
CHEB / 7.2189000e-02 -5.2645000e-07 -3.6644000e-07 /

CH3O+OH(+m)=sSPC(1735)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
45.28525416771308 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0261000e+01 1.9614000e+00 -2.6213000e-02 /
CHEB / -1.1490000e+00 1.4962000e-02 1.0261000e-02 /
CHEB / -7.5800000e-01 1.6474000e-02 1.1072000e-02 /
CHEB / -3.2104000e-01 4.6052000e-03 3.0811000e-03 /
CHEB / -1.0410000e-01 -1.0023000e-03 -6.5316000e-04 /

CH2OOH+H(+m)=CH3O+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -50.514375058605886
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4091000e+01 -8.4368000e-06 -5.8726000e-06 /
CHEB / -2.4726000e-01 3.3006000e-06 2.2974000e-06 /
CHEB / 2.8954000e-02 3.7516000e-06 2.6114000e-06 /
CHEB / 6.6845000e-02 8.6034000e-07 5.9886000e-07 /
CHEB / 4.2661000e-02 -4.5026000e-07 -3.1341000e-07 /

!CH3+HO2(+m)=CH3O+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -21.74764721929838
kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 1.3100000e+01 -1.0636000e-04 -7.4028000e-05 /
!CHEB / 3.3976000e-02 6.3601000e-05 4.4268000e-05 /
!CHEB / 1.2320000e-02 4.9957000e-05 3.4770000e-05 /
!CHEB / 4.3016000e-02 3.5531000e-06 2.4732000e-06 /
!CHEB / 2.3099000e-02 -1.0350000e-05 -7.2031000e-06 /

sSPC(1697)+H(+m)=sSPC(1735)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
85.09098360006828 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1688000e+00 2.0000000e+00 -1.2005000e-05 /
CHEB / -7.4725000e-01 6.5832000e-06 4.5824000e-06 /
CHEB / -3.0463000e-01 7.6360000e-06 5.3151000e-06 /
CHEB / -7.9293000e-02 1.8258000e-06 1.2709000e-06 /
CHEB / 5.3059000e-04 -8.6768000e-07 -6.0396000e-07 /
```

```
CH2OOH+H(+m)=sSPC(1697)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -10.708645626250679
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7500000e+00 -7.6496000e-06 -5.3247000e-06 /
CHEB / -6.3862000e-01 3.9528000e-06 2.7514000e-06 /
CHEB / 1.5521000e-01 3.3307000e-06 2.3184000e-06 /
CHEB / 1.1343000e-01 3.3805000e-07 2.3531000e-07 /
CHEB / 4.1710000e-02 -5.8390000e-07 -4.0643000e-07 /

sSPC(1697)+H(+m)=CH3+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -18.058082213056824
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1011000e+01 -1.5633000e-05 -1.0882000e-05 /
CHEB / 4.5402000e-02 8.1798000e-06 5.6937000e-06 /
CHEB / 2.4331000e-01 7.1293000e-06 4.9625000e-06 /
CHEB / 1.4332000e-01 8.4244000e-07 5.8640000e-07 /
CHEB / 5.7681000e-02 -1.2657000e-06 -8.8097000e-07 /

sSPC(1697)+H(+m)=CH3O+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (sSPC(1735))   deltaHrxn(T=298K) = -39.80572943235521
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3207000e+01 -1.6490000e-05 -1.1478000e-05 /
CHEB / -4.0953000e-01 7.4366000e-06 5.1764000e-06 /
CHEB / -2.8268000e-03 7.5717000e-06 5.2704000e-06 /
CHEB / 4.4762000e-02 1.4573000e-06 1.0144000e-06 /
CHEB / 2.5823000e-02 -1.0646000e-06 -7.4101000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+CH3C[O]cHCH3(+m)=sSPC(752)+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #11 (C7H12O4(372))
      deltaHrxn(T=298K) = -3.0501044063866827 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8142000e+00 -2.2224000e-01 -1.2084000e-01 /
CHEB / 3.2807000e+00 2.4903000e-01 1.2776000e-01 /
CHEB / 7.2928000e-01 -1.6213000e-02 -2.5795000e-03 /
CHEB / 9.3720000e-02 -3.9276000e-02 -2.0956000e-02 /
CHEB / -2.7012000e-02 3.5896000e-04 -2.0551000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+HO2(+m)=nSPC(879)+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C3H6O5JJ(343)) deltaHrxn(T=298K) = -
2.529759081387745 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5461000e+00 -1.2474000e-05 -8.6826000e-06 /
CHEB / 3.5286000e+00 -2.3559000e-05 -1.6398000e-05 /
CHEB / -4.7964000e-02 -2.0060000e-05 -1.3963000e-05 /
CHEB / 4.0295000e-02 -1.5663000e-05 -1.0902000e-05 /
CHEB / 4.0761000e-03 -1.1328000e-05 -7.8848000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+CH2C[O]CH3(+m)=sSPC(1590)+sSPC(1590)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #34 (C6H10O4(473))
      deltaHrxn(T=298K) = -30.12635487292117 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2440000e+01 -3.3037000e-01 -1.6339000e-01 /
CHEB / 2.0655000e-01 3.3190000e-01 1.5101000e-01 /
CHEB / -2.6087000e-02 2.3540000e-02 1.8979000e-02 /
CHEB / -3.1653000e-02 -5.1739000e-02 -2.1128000e-02 /
CHEB / -1.6678000e-02 -9.8774000e-03 -7.5879000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CHcH2    -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!Here are the path reactions and their high-P limit kinetics:

MEKenol+CH2(+m)=CH3C[OH]CHcH2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #53 (C5H10OJJ(650))      deltaHrxn(T=298K) = -
21.42786265489979 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0567000e+01 -4.9437000e-03 -3.4317000e-03 /
CHEB / 1.2113000e+00 3.0623000e-03 2.1215000e-03 /
CHEB / 2.1285000e-01 -1.0562000e-03 -7.3105000e-04 /
CHEB / 7.3796000e-02 -7.2826000e-04 -5.0574000e-04 /
CHEB / 2.7956000e-02 -3.9986000e-05 -2.8083000e-05 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(116)+CH3(+m)=sSPC(1697)+CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #65 (C5H12O3(854))
      deltaHrxn(T=298K) = 3.7101152856602297 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3450000e+00 -8.1610000e-02 -5.1543000e-02 /
CHEB / 4.5923000e+00 9.7342000e-02 6.0353000e-02 /
CHEB / 7.9210000e-01 -1.2610000e-02 -6.9237000e-03 /
CHEB / 1.6451000e-01 -1.4520000e-02 -9.2199000e-03 /
CHEB / 1.8527000e-02 2.7870000e-03 1.3908000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(332)+CH3(+m)=sSPC(1697)+CH3CH[OH]CH2CH2(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #66 (C5H12O3(1351))
      deltaHrxn(T=298K) = 1.9902393731799748 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6750000e+00 -4.0746000e-02 -2.7096000e-02 /
CHEB / 3.9786000e+00 4.6456000e-02 3.0619000e-02 /
CHEB / 8.6334000e-01 -4.5353000e-03 -2.8319000e-03 /
CHEB / 2.0265000e-01 -8.6576000e-03 -5.7320000e-03 /
CHEB / 3.3377000e-02 3.3798000e-04 1.1534000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+C4H7-24(+m)=CH3CH[o]C2H3+CH3O(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #79 (C5H10O2(926))
      deltaHrxn(T=298K) = -20.29782413360529 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3545000e+01 -4.4618000e-02 -3.3671000e-02 /
CHEB / -7.5547000e-01 5.2444000e-02 3.9764000e-02 /
CHEB / -3.9218000e-02 2.7101000e-03 1.4688000e-03 /
CHEB / -2.1140000e-02 -1.2727000e-02 -9.0112000e-03 /
CHEB / -1.7843000e-02 -1.8622000e-04 -2.0881000e-04 /
```

```
sSPC(46)+CH3(+m)=CH3CH[o]C2H3+CH3O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #79 (C5H10O2(926)) deltaHrxn(T=298K) = -
30.97634848893799 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4124000e+01 -9.9881000e-04 -8.4273000e-04 /
CHEB / -8.0709000e-01 8.5295000e-04 7.2121000e-04 /
CHEB / 8.8228000e-03 6.3568000e-04 5.3390000e-04 /
CHEB / 4.7328000e-02 -4.6453000e-04 -3.9215000e-04 /
CHEB / 2.3168000e-02 -1.8572000e-04 -1.5504000e-04 /

sSPC(46)+CH3(+m)=sSPC(1697)+C4H7-24(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #79 (C5H10O2(926)) deltaHrxn(T=298K) = -
10.678524355332698 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0239000e+01 -9.0228000e-03 -6.2529000e-03 /
CHEB / 8.5836000e-01 1.0539000e-02 7.3023000e-03 /
CHEB / 5.0150000e-01 1.4099000e-04 9.6661000e-05 /
CHEB / 1.5287000e-01 -1.8247000e-03 -1.2578000e-03 /
CHEB / 4.6995000e-02 -9.9395000e-05 -7.2690000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+CH3(+m)=sSPC(1697)+C4H7-24(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #108 (C5H10O2(1032))     deltaHrxn(T=298K) = -
12.248351181937323 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2090000e+00 -5.9913000e-03 -4.1683000e-03 /
CHEB / 1.6975000e+00 6.5151000e-03 4.5336000e-03 /
CHEB / 5.8674000e-01 8.6755000e-04 6.0133000e-04 /
CHEB / 1.8753000e-01 -1.3946000e-03 -9.6876000e-04 /
CHEB / 5.5519000e-02 -2.4967000e-04 -1.7333000e-04 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH3C[O]cHCH3+sSPC(1697)(+m)=sSPC(752)+CH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #137 (C5H10O3(420))
      deltaHrxn(T=298K) = -1.9900965525740943 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8137000e+00 -1.6455000e-02 -1.1264000e-02 /
CHEB / 3.3938000e+00 1.6896000e-02 1.1520000e-02 /
CHEB / 8.4180000e-01 -1.1871000e-03 -7.9645000e-04 /
CHEB / 1.7544000e-01 -4.0145000e-03 -2.7402000e-03 /
CHEB / 5.9560000e-03 -6.4901000e-04 -4.6206000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+CH2C[O]CH3(+m)=sSPC(1590)+CH3O(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O3(334))  deltaHrxn(T=298K)
= -29.916340697382207 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3256000e+01 -3.4342000e-02 -2.3125000e-02 /
CHEB / -5.0838000e-01 3.3626000e-02 2.2610000e-02 /
CHEB / -3.6232000e-02 7.4507000e-03 4.9212000e-03 /
CHEB / -3.9730000e-03 -8.0072000e-03 -5.2570000e-03 /
CHEB / -1.4020000e-02 -2.2170000e-03 -1.4832000e-03 /

sSPC(1356)+CH3(+m)=sSPC(1590)+CH3O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3(334))   deltaHrxn(T=298K) = -
30.976348551194793 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3966000e+01 -3.4342000e-02 -2.3125000e-02 /
CHEB / -6.7526000e-01 3.3626000e-02 2.2610000e-02 /
CHEB / 1.1676000e-02 7.4507000e-03 4.9212000e-03 /
CHEB / 4.1769000e-02 -8.0072000e-03 -5.2570000e-03 /
CHEB / 2.0838000e-02 -2.2170000e-03 -1.4832000e-03 /

sSPC(1697)+CH2C[O]CH3(+m)=sSPC(1356)+CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O3(334))  deltaHrxn(T=298K)
= 1.0600078538125857 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4767000e+00 -1.5134000e-02 -1.0354000e-02 /
CHEB / 3.1338000e+00 1.7293000e-02 1.1800000e-02 /
CHEB / 7.3881000e-01 -4.6933000e-04 -2.9687000e-04 /
CHEB / 1.5041000e-01 -2.9406000e-03 -2.0019000e-03 /
CHEB / 1.7147000e-02 -1.8081000e-04 -1.3672000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3O-2           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
sSPC(1909)+H(+m)=CH2CO+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #23 (C2H3O2J(455))      deltaHrxn(T=298K) = -
48.63508511328079 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2750000e+01 -1.2750000e-04 -8.9528000e-05 /
CHEB / -3.9375000e-01 1.0088000e-05 7.3701000e-06 /
CHEB / -1.0497000e-01 9.9994000e-05 7.0275000e-05 /
CHEB / 1.7354000e-02 4.1034000e-05 2.8562000e-05 /
CHEB / 2.3125000e-02 -7.7828000e-06 -5.6475000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+sSPC(1590)(+m)=CH2CO+sSPC(1356)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #75 (C5H7O4J(426))
      deltaHrxn(T=298K) = -8.619341505386618 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1777000e+01 -8.0265000e-01 -1.4645000e-01 /
CHEB / 6.2107000e-01 9.3807000e-01 1.1460000e-01 /
CHEB / -1.3266000e-01 1.5278000e-02 8.3089000e-02 /
CHEB / -1.1565000e-01 -1.3873000e-01 -2.5054000e-02 /
CHEB / -2.1328000e-02 -5.3110000e-02 -3.5212000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+CH3C[OH]CHcH2(+m)=CH3CO+C4H6O(717)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #173 (C6H9O2J(656))
      deltaHrxn(T=298K) = -10.758668712534682 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3655000e+00 -8.2062000e-05 -5.7113000e-05 /
CHEB / 1.4605000e+01 -1.0906000e-04 -7.5899000e-05 /
CHEB / 3.3859000e-01 -9.9864000e-05 -6.9497000e-05 /
CHEB / 1.1969000e-01 -8.9252000e-05 -6.2112000e-05 /
CHEB / 3.8049000e-02 -6.9429000e-05 -4.8316000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+CH3C[O]cHCH3(+m)=CH2CO+MEKenol(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #249 (C6H10O2(832))      deltaHrxn(T=298K) = -
44.95551683239858 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4949000e+00 -1.1441000e+00 -8.2524000e-02 /
```

```
CHEB / 3.1331000e+00 1.1275000e+00 -8.8616000e-03 /
CHEB / 2.3643000e-01 2.5967000e-01 1.0277000e-01 /
CHEB / -1.0417000e-01 -1.3488000e-01 4.4720000e-02 /
CHEB / -3.8980000e-02 -1.2558000e-01 -2.7886000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+CH3O(+m)=CH2CO+sSPC(1697)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #364 (C3H5O3J(428))      deltaHrxn(T=298K) = -
8.82935568092558 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1933000e+01 -3.7127000e-01 -1.5809000e-01 /
CHEB / 1.2354000e-01 4.3631000e-01 1.7452000e-01 /
CHEB / -3.6248000e-02 -7.0068000e-03 1.0653000e-02 /
CHEB / -3.0513000e-02 -5.4570000e-02 -1.9875000e-02 /
CHEB / 8.8640000e-03 -1.1820000e-02 -9.9717000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+CH3(+m)=CH3O+CH3O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #629 (C2H6O2(344))      deltaHrxn(T=298K) = -
30.766334375655827 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3882000e+01 2.1245000e-09 1.4783000e-09 /
CHEB / -6.1045000e-01 3.5307000e-09 2.4579000e-09 /
CHEB / 1.1610000e-02 2.0607000e-09 1.4348000e-09 /
CHEB / 4.1955000e-02 6.8561000e-10 4.7723000e-10 /
CHEB / 2.1665000e-02 -1.2680000e-10 -8.8443000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!Here are the path reactions and their high-P limit kinetics:

CH2OOH+OCOOH(+m)=nSPC(801)+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #652 (C2H4O5(1290))     deltaHrxn(T=298K) = -
25.54700865611004 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0280000e+01 -8.8909000e-04 -6.1926000e-04 /
CHEB / 6.9537000e-01 9.4071000e-04 6.5526000e-04 /
CHEB / 2.9900000e-01 1.2535000e-04 8.7267000e-05 /
CHEB / 1.2165000e-01 -1.5451000e-04 -1.0765000e-04 /
CHEB / 3.4777000e-02 -4.8438000e-05 -3.3718000e-05 /

nSPC(879)+H(+m)=CH2OOH+OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #652 (C2H4O5(1290))     deltaHrxn(T=298K) =
6.778973372637189 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4595000e+00 -1.2922000e-03 -8.9846000e-04 /
CHEB / 4.6457000e+00 1.5633000e-03 1.0868000e-03 /
CHEB / 8.2445000e-01 -1.0162000e-04 -7.0433000e-05 /
CHEB / 2.2563000e-01 -1.9105000e-04 -1.3283000e-04 /
CHEB / 6.0043000e-02 -8.0360000e-06 -5.6634000e-06 /

nSPC(879)+H(+m)=nSPC(801)+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #652 (C2H4O5(1290))     deltaHrxn(T=298K) = -
18.76803528347285 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0592000e+01 -2.2585000e-03 -1.5735000e-03 /
CHEB / 4.1498000e-01 2.5765000e-03 1.7952000e-03 /
CHEB / 3.4782000e-01 9.5248000e-05 6.6081000e-05 /
CHEB / 1.2614000e-01 -4.2290000e-04 -2.9468000e-04 /
CHEB / 3.5599000e-02 -6.3205000e-05 -4.3928000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
```

```
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

nSPC(879)+CH3CH[OH]CHCH3(+m)=sSPC(116)+nSPC(801)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #707 (C6H12O6(1386))
      deltaHrxn(T=298K) = -4.420068356076257 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4566000e+00 -2.7596000e-01 -1.4014000e-01 /
CHEB / 3.2116000e+00 3.1730000e-01 1.4978000e-01 /
CHEB / 7.7452000e-01 -2.4163000e-02 -1.3645000e-03 /
CHEB / 8.1260000e-02 -4.2964000e-02 -2.1299000e-02 /
CHEB / -2.4272000e-02 7.4781000e-03 9.4480000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(46)+nSPC(801)(+m)=nSPC(879)+C4H7-24(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #786 (C6H10O5(1547))
      deltaHrxn(T=298K) = -9.968571284916663 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9209000e+00 -1.1299000e-01 -6.8561000e-02 /
CHEB / 1.6729000e+00 1.4462000e-01 8.6207000e-02 /
CHEB / 5.0376000e-01 -1.6854000e-02 -7.7316000e-03 /
CHEB / 7.7556000e-02 -1.9287000e-02 -1.2178000e-02 /
CHEB / -1.3879000e-02 4.8676000e-04 -4.2375000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+nSPC(801)(+m)=nSPC(879)+C4H7-24(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #907 (C6H10O5(1691))
      deltaHrxn(T=298K) = -11.538398111521296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1155000e+00 -1.7540000e-01 -1.0020000e-01 /
CHEB / 1.7888000e+00 2.1776000e-01 1.2112000e-01 /
CHEB / 4.2100000e-01 -1.5581000e-02 -3.9709000e-03 /
CHEB / 7.2371000e-02 -3.1204000e-02 -1.8075000e-02 /
CHEB / -2.0377000e-03 -2.6776000e-03 -3.4259000e-03 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(879)+CH3C[O]cHCH3(+m)=nSPC(801)+sSPC(752)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1036 (C6H10O6(1295))
      deltaHrxn(T=298K) = -2.7000496229901287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9632000e+00 -2.5561000e-01 -1.2887000e-01 /
CHEB / 3.5892000e+00 3.2547000e-01 1.5681000e-01 /
CHEB / 6.7458000e-01 -3.4375000e-02 -5.6046000e-03 /
CHEB / 5.6106000e-02 -4.5342000e-02 -2.4889000e-02 /
CHEB / -4.0069000e-02 1.2352000e-05 -3.7317000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
```

```
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

nSPC(879)+CH3CH[OH]CH2CH2(+m)=sSPC(332)+nSPC(801)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C6H12O6(356)) deltaHrxn(T=298K)
= -2.700192443596002 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3751000e+00 -2.4628000e-01 -1.2562000e-01 /
CHEB / 3.9793000e+00 3.1587000e-01 1.5426000e-01 /
CHEB / 7.2499000e-01 -3.6137000e-02 -7.1722000e-03 /
CHEB / 5.3334000e-02 -4.3920000e-02 -2.4675000e-02 /
CHEB / -4.1711000e-02 8.4208000e-04 -3.0648000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+nSPC(879)(+m)=sSPC(1356)+nSPC(801)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2 (C5H8O6(447))  deltaHrxn(T=298K)
= 0.3500547833965655 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1133000e+00 -5.9946000e-02 -3.8964000e-02 /
CHEB / 3.4626000e+00 6.8687000e-02 4.4019000e-02 /
CHEB / 6.4919000e-01 -7.5052000e-03 -4.3926000e-03 /
CHEB / 1.0006000e-01 -1.1920000e-02 -7.7739000e-03 /
CHEB / -1.5215000e-02 -1.4592000e-04 -3.1556000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(879)+CH3(+m)=sSPC(1697)+nSPC(801)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C3H6O5(513))  deltaHrxn(T=298K)
= -0.7099530704160273 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6479000e+00 -1.2147000e-02 -8.3350000e-03 /
CHEB / 3.1917000e+00 1.4226000e-02 9.7398000e-03 /
CHEB / 7.0430000e-01 -9.8487000e-04 -6.5725000e-04 /
CHEB / 1.5532000e-01 -2.3913000e-03 -1.6373000e-03 /
CHEB / 2.7393000e-02 7.8513000e-05 4.5318000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+CH3(+m)=CH2CO+CH3O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #28 (C3H5O2J(582))      deltaHrxn(T=298K) = -
39.595690056581404 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2806000e+01 -1.3599000e-02 -9.3723000e-03 /
CHEB / -1.0629000e-01 1.2909000e-02 8.8839000e-03 /
CHEB / -1.7824000e-03 3.1135000e-03 2.1507000e-03 /
CHEB / 4.5076000e-02 -1.8187000e-03 -1.2425000e-03 /
CHEB / 3.0547000e-02 -1.2234000e-03 -8.4388000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     C3H5OJ      27.09 76.26 18.34 21.54 24.52 27.2  31.62 34.9  39.89
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C3H5OJ(17)  19.42 73.31 19.06 22.62 25.73 28.35 32.45 35.48 40.34
      null
!Here are the path reactions and their high-P limit kinetics:

C3H5OJ+O(+m)=CH2OH+CH2CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
101.5596474230429 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3378000e+01 2.3264000e-04 1.6191000e-04 /
CHEB / -8.7569000e-01 -1.6808000e-04 -1.1697000e-04 /
CHEB / -2.1915000e-01 -5.9444000e-05 -4.1373000e-05 /
CHEB / -1.0491000e-01 -1.2610000e-05 -8.7867000e-06 /
CHEB / -5.3423000e-02 3.0583000e-06 2.1263000e-06 /

C3H5OJ(17)+O(+m)=CH2OH+CH2CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
93.89035344541887 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1607000e+01 6.9179000e-03 4.8785000e-03 /
CHEB / -4.7632000e-01 -8.2514000e-03 -5.8370000e-03 /
CHEB / -3.7929000e-01 5.2564000e-04 3.9700000e-04 /
CHEB / -1.8299000e-01 9.5871000e-04 6.7217000e-04 /
CHEB / -7.5051000e-02 -2.8507000e-05 -2.6348000e-05 /

C3H5OJ+O(+m)=C3H5OJ(17)+O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
7.669293977624029 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9290000e+00 -8.3130000e-03 -5.7684000e-03 /
CHEB / 2.3379000e+00 1.0001000e-02 6.9380000e-03 /
CHEB / 7.6781000e-01 -4.5673000e-04 -3.1666000e-04 /
CHEB / 1.6789000e-01 -1.4543000e-03 -1.0062000e-03 /
CHEB / 5.1555000e-02 5.1077000e-05 3.3846000e-05 /

CH2OH+CH2CO(+m)=sSPC(1590)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
17.767476758438306 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3534000e+00 -8.1875000e-01 -1.4830000e-01 /
CHEB / 4.6387000e+00 9.1215000e-01 1.0754000e-01 /
CHEB / 9.1734000e-02 4.5422000e-02 7.6961000e-02 /
CHEB / -6.4850000e-02 -1.1169000e-01 -5.8489000e-03 /
CHEB / -1.2259000e-02 -4.1423000e-02 -2.5895000e-02 /

C3H5OJ+O(+m)=sSPC(1590)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
119.32712418148121 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0889000e+01 2.3212000e-04 1.6168000e-04 /
CHEB / -2.5306000e-01 -1.6369000e-04 -1.1407000e-04 /
CHEB / -4.8489000e-02 -7.0187000e-05 -4.8867000e-05 /
CHEB / -4.4679000e-02 -8.9507000e-06 -6.1729000e-06 /
CHEB / -2.9617000e-02 7.5788000e-06 5.2667000e-06 /

C3H5OJ(17)+O(+m)=sSPC(1590)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #106 (C3H5O2J(803))     deltaHrxn(T=298K) = -
111.65783020385717 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.1449000e+01 3.4887000e-03 2.4437000e-03 /
CHEB / -2.9729000e-01 -4.5208000e-03 -3.1721000e-03 /
CHEB / -6.8765000e-02 6.5414000e-04 4.6808000e-04 /
CHEB / -9.7045000e-03 5.4345000e-04 3.7653000e-04 /
CHEB / 2.5992000e-03 -9.2152000e-05 -6.6031000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO              -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3O               4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     H                  49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3                34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                 -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O               4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2OH              -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH2O               -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                  49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3                34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     O                  59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+H=CH3O              1.0000000e+11      0.00000
1.1900000e+04
!     CH3O=CH2OH                     1.8288499e+09      1.13906
3.4790987e+04
!     CH3+O=CH3O               1.0000000e+13      0.00000
0.0000000e+00

CH3+O(+m)=CH3O(+m)      1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#289 (CH3O) High-P Limit: Oa_R_Recombination estimate: (Average:)
C_methyl     Oa         deltaHrxn(T=298K) = -90.18019994485442 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0768000e+01 1.9292000e+00 -4.6171000e-02 /
CHEB / -1.8009000e+00 8.9906000e-02 5.7828000e-02 /
```

```
CHEB / -4.8247000e-01 -1.4631000e-02 -8.2202000e-03 /
CHEB / -1.2170000e-01 -5.1982000e-03 -3.8623000e-03 /
CHEB / -1.2287000e-02 -2.3528000e-04 -2.5508000e-04 /

CH3+O(+m)=CH2O+H(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#289 (CH3O) deltaHrxn(T=298K) = -71.30280672512123 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3839000e+00 -7.0712000e-02 -4.6117000e-02 /
CHEB / -2.7938000e+00 8.9930000e-02 5.7847000e-02 /
CHEB / -6.2614000e-01 -1.4696000e-02 -8.2637000e-03 /
CHEB / -1.7710000e-01 -5.2408000e-03 -3.8924000e-03 /
CHEB / -5.8653000e-02 -2.3570000e-04 -2.5587000e-04 /

CH3O(+m)=CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#289 (CH3O) High-P Limit: intra_H_migration estimate: (Average:) Others-
R2H_S    O_rad_out     Cs_H_out_2H        deltaHrxn(T=298K) = -
7.759401965243102 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9758000e+00 1.1475000e+00 -2.4425000e-01 /
CHEB / 1.0997000e+01 6.9154000e-01 1.1869000e-01 /
CHEB / -5.5089000e-01 1.8261000e-01 9.9604000e-02 /
CHEB / -2.9194000e-01 1.1871000e-02 3.1413000e-02 /
CHEB / -1.2286000e-01 -2.9443000e-02 -3.6902000e-03 /

CH3+O(+m)=CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#289 (CH3O) deltaHrxn(T=298K) = -97.93960191009752 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3564000e+01 -7.0707000e-02 -4.6114000e-02 /
CHEB / -3.8939000e-01 8.9932000e-02 5.7849000e-02 /
CHEB / 9.1785000e-03 -1.4700000e-02 -8.2667000e-03 /
CHEB / 4.6562000e-02 -5.2438000e-03 -3.8945000e-03 /
CHEB / 2.9606000e-02 -2.3582000e-04 -2.5599000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
CH3+sSPC(1590)(+m)=CH3O+CH2C[O]CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #317 (C4H8O2(587)) deltaHrxn(T=298K) = -
0.8499936782736253 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5676000e+00 -1.3548000e+00 -4.9776000e-02 /
CHEB / 2.8544000e+00 1.0263000e+00 -4.3909000e-02 /
CHEB / 2.7234000e-01 4.7937000e-01 4.2140000e-02 /
CHEB / -2.1792000e-01 4.9336000e-02 6.1075000e-02 /
CHEB / -1.4192000e-01 -1.1076000e-01 2.2680000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(801)+O(+m)=CH2O+OCOOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #379 (C2H3O4J(392))     deltaHrxn(T=298K) = -
74.52252590831867 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3414000e+01 1.8108000e-08 1.2605000e-08 /
CHEB / -3.5299000e-01 2.3427000e-08 1.6307000e-08 /
CHEB / -1.6649000e-02 1.3508000e-08 9.4023000e-09 /
CHEB / 5.5743000e-03 8.5979000e-09 5.9848000e-09 /
CHEB / -4.4030000e-03 6.1186000e-09 4.2590000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
```

```
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+O=sSPC(1909)      2.3501400e+11      0.30815
4.9629937e+03
!     CH2+CO2=sSPC(1909)      2.3501400e+11      0.30815
4.9629937e+03

CH2CO+O(+m)=sSPC(1909)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #491 (sSPC(1909)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Cd/H2     Y_rad_birad         deltaHrxn(T=298K)
= -50.58450988827302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.1407000e+00 2.0070000e+00 4.8400000e-03 /
CHEB / -3.2278000e-01 -7.8839000e-04 -5.4856000e-04 /
CHEB / -8.6814000e-01 -2.8329000e-04 -1.9711000e-04 /
CHEB / -4.0173000e-01 -8.3954000e-05 -5.8412000e-05 /
CHEB / -1.5992000e-01 -2.2703000e-05 -1.5794000e-05 /

sSPC(1909)(+m)=CH2+CO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #491 (sSPC(1909)) deltaHrxn(T=298K) = 0.6695034107172546
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5162000e+00 1.9998000e+00 -1.2625000e-04 /
CHEB / 2.1506000e+00 5.4795000e-05 3.8143000e-05 /
CHEB / -9.8128000e-01 1.9792000e-05 1.3777000e-05 /
CHEB / -4.5030000e-01 5.2621000e-06 3.6621000e-06 /
CHEB / -1.7345000e-01 1.1334000e-06 7.8846000e-07 /

CH2CO+O(+m)=CH2+CO2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#491 (sSPC(1909)) deltaHrxn(T=298K) = -49.915006477555764 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0977000e+01 -6.0071000e-09 -4.1814000e-09 /
CHEB / 1.1669000e+00 6.7364000e-09 4.6891000e-09 /
CHEB / 2.2112000e-02 5.4479000e-09 3.7922000e-09 /
CHEB / 1.2105000e-02 2.3584000e-09 1.6416000e-09 /
CHEB / -2.2592000e-03 7.0626000e-10 4.9161000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
```

```
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+CH2C[O]CH3(+m)=CH2CO+sSPC(1590)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #687 (C5H7O3J(660))
      deltaHrxn(T=298K) = -38.745696378307784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2362000e+01 -3.7770000e-01 -1.7973000e-01 /
CHEB / 3.4931000e-02 4.0377000e-01 1.7702000e-01 /
CHEB / -2.7271000e-02 3.8761000e-02 3.4393000e-02 /
CHEB / -5.2301000e-02 -5.4045000e-02 -2.1271000e-02 /
CHEB / -3.7487000e-02 -2.6994000e-02 -1.7614000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H6O(717)+sSPC(2810)(+m)=CH3C[O]cHCH3+CO2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #949 (C5H7O3J(1717))
      deltaHrxn(T=298K) = -36.126516292401256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5545000e+00 -4.3076000e-01 -2.1194000e-01 /
```

```
CHEB / 1.2969000e+01 4.5287000e-01 2.0383000e-01 /
CHEB / -3.3836000e-01 7.2869000e-02 5.5430000e-02 /
CHEB / -2.8744000e-01 -6.1559000e-02 -2.0565000e-02 /
CHEB / -1.4485000e-01 -4.7749000e-02 -2.8445000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+sSPC(1909)(+m)=CO2+CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1472 (C4H5O3J(885))     deltaHrxn(T=298K) = -
92.29067806147359 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8747000e+00 -2.1063000e-04 -1.4660000e-04 /
CHEB / 2.1601000e+00 2.4955000e-04 1.7369000e-04 /
CHEB / 7.8903000e-01 -5.6522000e-06 -3.9324000e-06 /
CHEB / 2.0920000e-01 -3.7483000e-05 -2.6088000e-05 /
CHEB / 5.0634000e-02 -1.3840000e-06 -9.6412000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!Here are the path reactions and their high-P limit kinetics:

CO+sSPC(1590)(+m)=CO2+CH2C[O]CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1718 (C4H5O3J(846))     deltaHrxn(T=298K) = -
37.83644130908153 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3706000e+00 4.7511000e-11 3.3070000e-11 /
CHEB / 9.6263000e-01 9.3213000e-11 6.4885000e-11 /
CHEB / 2.8849000e-03 8.7838000e-11 6.1140000e-11 /
CHEB / 3.4968000e-03 7.9053000e-11 5.5028000e-11 /
CHEB / 2.2124000e-03 6.7198000e-11 4.6774000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!Here are the path reactions and their high-P limit kinetics:

CO+CH3O(+m)=CO2+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1806 (C2H3O2J(848))    deltaHrxn(T=298K) = -36.98644763080791 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7972000e+00 -4.7653000e-06 -3.3170000e-06 /
CHEB / 6.7342000e-01 -9.2218000e-06 -6.4190000e-06 /
CHEB / 2.9688000e-02 -8.3525000e-06 -5.8139000e-06 /
CHEB / 5.0885000e-02 -7.0741000e-06 -4.9240000e-06 /
CHEB / 3.4471000e-02 -5.5809000e-06 -3.8847000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+O(+m)=CO2+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1904 (C2H3O2J(849))    deltaHrxn(T=298K) = -116.49831554779155 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3498000e+01 -1.3749000e-05 -9.5698000e-06 /
CHEB / -4.7895000e-01 -2.4297000e-05 -1.6912000e-05 /
CHEB / -5.3561000e-02 -1.7451000e-05 -1.2147000e-05 /
CHEB / -2.4000000e-02 -1.0813000e-05 -7.5263000e-06 /
CHEB / -2.3745000e-02 -5.8808000e-06 -4.0933000e-06 /

sSPC(1909)+H(+m)=CH3CO+O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1904 (C2H3O2J(849))    deltaHrxn(T=298K) =
10.649146526823799 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3812000e+00 -1.0836000e-05 -7.5426000e-06 /
CHEB / 6.2020000e+00 -1.8670000e-05 -1.2995000e-05 /
CHEB / 8.6661000e-01 -1.2378000e-05 -8.6157000e-06 /
CHEB / 2.6714000e-01 -6.5502000e-06 -4.5593000e-06 /
CHEB / 6.7805000e-02 -2.5559000e-06 -1.7790000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3O             4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

HCO+CH2O(+m)=CO+CH3O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2070 (C2H3O2J(975))    deltaHrxn(T=298K) = -
6.699169041531383 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5823000e+01 -9.3000000e-06 -6.4734000e-06 /
```

```
CHEB / 2.3478000e+01 -9.3129000e-06 -6.4824000e-06 /
CHEB / 3.3342000e-01 -4.9663000e-06 -3.4568000e-06 /
CHEB / 1.6598000e-01 -4.0692000e-06 -2.8324000e-06 /
CHEB / 8.2810000e-02 -3.5487000e-06 -2.4701000e-06 /

CH2CHO+O(+m)=HCO+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2070 (C2H3O2J(975))    deltaHrxn(T=298K) = -
81.38186902839111 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3642000e+01 -7.9061000e-06 -5.5032000e-06 /
CHEB / -5.5633000e-01 -8.0530000e-06 -5.6055000e-06 /
CHEB / -2.6020000e-02 -4.2910000e-06 -2.9868000e-06 /
CHEB / -8.3436000e-03 -3.4267000e-06 -2.3852000e-06 /
CHEB / -1.2590000e-02 -2.9444000e-06 -2.0495000e-06 /

CH2CHO+O(+m)=CO+CH3O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2070 (C2H3O2J(975))    deltaHrxn(T=298K) = -
88.08103806992249 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1512000e+00 -6.7236000e-06 -4.6801000e-06 /
CHEB / 1.9811000e+00 -5.9413000e-06 -4.1356000e-06 /
CHEB / 8.7420000e-01 -2.6334000e-06 -1.8330000e-06 /
CHEB / 2.7631000e-01 -2.1343000e-06 -1.4856000e-06 /
CHEB / 7.5368000e-02 -1.9323000e-06 -1.3450000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+CH2CO(+m)=CO2+CH3CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2243 (C3H3O3J(934))    deltaHrxn(T=298K) = -
46.685255421998505 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.9195000e-01 -6.6324000e-03 -4.5974000e-03 /
CHEB / 1.0650000e+01 5.5965000e-03 3.8736000e-03 /
CHEB / 3.3488000e-01 8.2805000e-04 5.7615000e-04 /
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CHEB / 1.2121000e-01 -7.6885000e-04 -5.3135000e-04 /
CHEB / 3.4109000e-02 -4.7827000e-04 -3.3220000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+HCO(+m)=CH2CO+sSPC(2810)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2554 (C3H3O3J(1117))    deltaHrxn(T=298K) = -
57.654021448638204 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3162000e+01 4.9467000e-08 3.4433000e-08 /
CHEB / -4.1938000e-01 8.5697000e-08 5.9651000e-08 /
CHEB / -2.3690000e-02 5.6525000e-08 3.9346000e-08 /
CHEB / 1.1944000e-02 2.6670000e-08 1.8565000e-08 /
CHEB / 7.1677000e-03 5.5960000e-09 3.8953000e-09 /

CH2CO+sSPC(2810)(+m)=CH2CHO+CO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2554 (C3H3O3J(1117))   deltaHrxn(T=298K) = -
38.11608526905967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1214000e+00 2.3466000e-08 1.6334000e-08 /
CHEB / 1.3634000e+01 4.1078000e-08 2.8593000e-08 /
CHEB / 2.7151000e-01 3.0952000e-08 2.1545000e-08 /
CHEB / 1.0196000e-01 2.1146000e-08 1.4719000e-08 /
CHEB / 3.6733000e-02 1.2996000e-08 9.0459000e-09 /

sSPC(1909)+HCO(+m)=CH2CHO+CO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2554 (C3H3O3J(1117))   deltaHrxn(T=298K) = -
95.77010671769787 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7065000e+00 -2.9702000e-05 -2.0675000e-05 /
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CHEB / 1.4632000e+00 2.3986000e-05 1.6696000e-05 /
CHEB / 6.3465000e-01 8.8549000e-06 6.1637000e-06 /
CHEB / 2.2236000e-01 -1.6043000e-06 -1.1167000e-06 /
CHEB / 8.0578000e-02 -1.5700000e-06 -1.0928000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+CH3CH[OH]CHCH3(+m)=CO2+sBuOH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2840 (C5H10O3(1017))
      deltaHrxn(T=298K) = -102.08973124473948 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7125000e+00 -1.4584000e+00 -4.2220000e-02 /
CHEB / 2.1546000e+00 9.3448000e-01 -5.2319000e-02 /
CHEB / 3.0877000e-01 5.7817000e-01 1.3276000e-02 /
CHEB / -2.7478000e-01 2.0289000e-01 5.6468000e-02 /
CHEB / -2.7563000e-01 -4.4586000e-02 5.0918000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-2          -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2              -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     C3H6             4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+CH3CH[OH]CH2CH2(+m)=CO2+sBuOH(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2957 (C5H10O3(1018))
      deltaHrxn(T=298K) = -104.73938959682988 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0024000e+01 -1.4169000e+00 -4.3555000e-02 /
CHEB / 1.7968000e+00 9.8507000e-01 -4.6471000e-02 /
CHEB / 1.4586000e-01 5.6639000e-01 2.9523000e-02 /
CHEB / -3.1640000e-01 1.5321000e-01 6.7575000e-02 /
CHEB / -2.7623000e-01 -8.9542000e-02 4.4136000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3CH[o]C2H3     12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     C4H7-24          32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H8-1            -0.11 73.61 20.57 26.09 31.04 35.28 41.96 46.97
      54.75 null
!Here are the path reactions and their high-P limit kinetics:

HCO+CH3CH[o]C2H3(+m)=sSPC(2810)+C4H7-24(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3128 (C5H8O2(1231))
      deltaHrxn(T=298K) = -28.526841634107328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2397000e+01 -1.1102000e+00 -1.6890000e-01 /
CHEB / -1.6470000e-01 8.9857000e-01 3.3382000e-02 /
CHEB / 1.1124000e-01 3.0510000e-01 9.0876000e-02 /
CHEB / -1.1245000e-01 -1.1184000e-02 5.4257000e-02 /
CHEB / -1.1164000e-01 -7.7297000e-02 1.3679000e-03 /

HCO+CH3CH[o]C2H3(+m)=CO+sC4H8O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3128 (C5H8O2(1231))    deltaHrxn(T=298K) = -
88.77101120453736 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0188000e+01 -1.1364000e+00 -1.6783000e-01 /
CHEB / 1.1678000e+00 8.8887000e-01 2.5255000e-02 /
CHEB / 4.2744000e-01 3.2272000e-01 8.5947000e-02 /
CHEB / 1.0477000e-02 3.1522000e-03 5.7607000e-02 /
CHEB / -5.9261000e-02 -7.3409000e-02 6.2155000e-03 /

sSPC(2810)+C4H7-24(+m)=CO+sC4H8O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3128 (C5H8O2(1231))     deltaHrxn(T=298K) = -
60.24416957043003 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7567000e+00 -1.4674000e+00 -6.6012000e-02 /
CHEB / 3.4672000e+00 8.8984000e-01 -8.3619000e-02 /
CHEB / 6.8686000e-01 5.0060000e-01 6.8169000e-03 /
CHEB / -9.1943000e-02 1.4341000e-01 5.7575000e-02 /
CHEB / -1.4577000e-01 -4.3804000e-02 4.7824000e-02 /

HCO+CH3CH[o]C2H3(+m)=CO2+C4H8-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3128 (C5H8O2(1231))    deltaHrxn(T=298K) = -
117.25780339716128 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2264000e+01 -1.1511000e+00 -1.6762000e-01 /
CHEB / 4.1947000e-02 8.8150000e-01 2.0620000e-02 /
CHEB / 1.0376000e-01 3.3165000e-01 8.2838000e-02 /
CHEB / -9.8639000e-02 1.1814000e-02 5.9130000e-02 /
CHEB / -1.0009000e-01 -7.0272000e-02 8.9929000e-03 /

sSPC(2810)+C4H7-24(+m)=CO2+C4H8-1(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3128 (C5H8O2(1231))     deltaHrxn(T=298K) = -
88.73096176305395 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0199000e+01 -1.4885000e+00 -6.4242000e-02 /
CHEB / 2.0014000e+00 8.6462000e-01 -8.5081000e-02 /
CHEB / 3.6872000e-01 5.0554000e-01 -8.3829000e-04 /
CHEB / -1.8841000e-01 1.6311000e-01 5.1521000e-02 /
CHEB / -1.8816000e-01 -2.9365000e-02 4.8168000e-02 /

CO+sC4H8O(+m)=CO2+C4H8-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3128 (C5H8O2(1231))    deltaHrxn(T=298K) = -
28.48679219262392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5258000e+01 -1.5306000e+00 -5.8927000e-02 /
CHEB / 2.2333000e+01 8.1317000e-01 -8.5270000e-02 /
CHEB / 9.2806000e-01 5.1350000e-01 -1.5776000e-02 /
CHEB / -2.1816000e-02 2.0229000e-01 3.7222000e-02 /
CHEB / -1.3226000e-01 1.3514000e-03 4.6236000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

HCO+CH3C[OH]CHcH2(+m)=CO+sC4H8O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3393 (C5H8O2(1873))    deltaHrxn(T=298K) = -
65.48323768377719 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8416000e+00 -8.9921000e-01 -1.5984000e-01 /
CHEB / 5.9475000e+00 9.3792000e-01 9.9756000e-02 /
CHEB / 1.5309000e-01 1.3145000e-01 9.4655000e-02 /
CHEB / -6.7253000e-02 -1.1128000e-01 8.3174000e-03 /
CHEB / -2.9093000e-02 -7.1042000e-02 -3.1693000e-02 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3C[OH]cH  20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23 39.84
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+CH3C[OH]cH(+m)=HCO+CH3C[OH]CHcH2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3674 (C5H8O2(2010))
      deltaHrxn(T=298K) = -26.75744947973009 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2287000e+01 -7.2510000e-01 -2.1334000e-01 /
CHEB / 3.4684000e-01 7.0348000e-01 1.6445000e-01 /
CHEB / 2.7683000e-02 1.4448000e-01 7.8771000e-02 /
CHEB / -8.3080000e-02 -6.3707000e-02 3.9878000e-03 /
CHEB / -6.5658000e-02 -5.7681000e-02 -2.3750000e-02 /

HCO+CH3C[OH]CHcH2(+m)=CO+MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3674 (C5H8O2(2010))     deltaHrxn(T=298K) = -
72.9125855985834 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0103000e+00 -1.1769000e+00 -1.0308000e-01 /
CHEB / 6.2200000e+00 1.0419000e+00 -5.8522000e-03 /
CHEB / 3.6884000e-01 3.0886000e-01 9.4927000e-02 /
CHEB / -3.4955000e-02 -4.4600000e-02 5.0629000e-02 /
CHEB / -4.2320000e-02 -1.0022000e-01 -7.1471000e-03 /

CH2CHO+CH3C[OH]cH(+m)=CO+MEKenol(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3674 (C5H8O2(2010))     deltaHrxn(T=298K) = -
99.6700350783135 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6169000e+00 -6.7303000e-01 -2.0759000e-01 /
CHEB / 2.2090000e+00 6.9007000e-01 1.7253000e-01 /
CHEB / 5.5129000e-01 9.9623000e-02 7.1706000e-02 /
CHEB / 8.1132000e-02 -7.2211000e-02 -6.5690000e-03 /
CHEB / -2.4985000e-03 -5.1302000e-02 -2.5710000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     C4H7-22           53.68 74.2  20.36 24.53 28.48 32.06 38.0  42.53
      49.64 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H8-2      -3.22 71.02 20.7  25.74 30.42 34.58 41.34 46.44 54.4
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+C4H7-22(+m)=HCO+CH3C[O]cHCH3(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3971 (C5H8O2(2011))
      deltaHrxn(T=298K) = -15.758674897860757 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2349000e+01 -8.3441000e-01 -2.0120000e-01 /
CHEB / 1.7368000e-01 8.3149000e-01 1.2771000e-01 /
CHEB / 1.5127000e-01 1.2562000e-01 9.5830000e-02 /
CHEB / -7.8892000e-02 -8.4821000e-02 5.0800000e-03 /
CHEB / -5.4596000e-02 -6.0090000e-02 -2.6712000e-02 /

HCO+CH3C[O]cHCH3(+m)=CO+MEKenol(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3971 (C5H8O2(2011))    deltaHrxn(T=298K) = -
72.71265601564596 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0318000e+01 -1.1915000e+00 -1.3067000e-01 /
CHEB / 1.6074000e+00 9.9956000e-01 -1.9087000e-02 /
CHEB / 2.4155000e-01 3.0825000e-01 9.9365000e-02 /
CHEB / -7.5728000e-02 -3.5200000e-02 6.5130000e-02 /
CHEB / -5.9451000e-02 -8.4935000e-02 2.2487000e-03 /

sSPC(2810)+C4H7-22(+m)=CO+MEKenol(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3971 (C5H8O2(2011))     deltaHrxn(T=298K) = -
88.47133091350673 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1340000e+01 -8.9637000e-01 -2.0628000e-01 /
```

```
CHEB / 5.9861000e-01 8.2968000e-01 1.0913000e-01 /
CHEB / 1.6813000e-01 1.7688000e-01 9.9999000e-02 /
CHEB / -3.9428000e-02 -6.2440000e-02 2.1061000e-02 /
CHEB / -3.0990000e-02 -6.4297000e-02 -1.9428000e-02 /

HCO+CH3C[O]cHCH3(+m)=CO2+C4H8-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3971 (C5H8O2(2011))    deltaHrxn(T=298K) = -
96.87984033217272 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1633000e+01 -1.2014000e+00 -1.3030000e-01 /
CHEB / 7.0312000e-01 9.9444000e-01 -2.2168000e-02 /
CHEB / -8.6145000e-03 3.1598000e-01 9.7108000e-02 /
CHEB / -1.5836000e-01 -2.8399000e-02 6.6774000e-02 /
CHEB / -9.1432000e-02 -8.3367000e-02 4.8743000e-03 /

sSPC(2810)+C4H7-22(+m)=CO2+C4H8-2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3971 (C5H8O2(2011))     deltaHrxn(T=298K) = -
112.63851523003349 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2567000e+01 -9.0215000e-01 -2.0708000e-01 /
CHEB / -2.3850000e-01 8.2787000e-01 1.0715000e-01 /
CHEB / -7.1912000e-02 1.8134000e-01 1.0013000e-01 /
CHEB / -1.2333000e-01 -5.9342000e-02 2.2647000e-02 /
CHEB / -6.3317000e-02 -6.3889000e-02 -1.8358000e-02 /

CO+MEKenol(+m)=CO2+C4H8-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3971 (C5H8O2(2011))    deltaHrxn(T=298K) = -
24.167184316526765 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4701000e+01 -1.4183000e+00 -7.0773000e-02 /
CHEB / 2.1983000e+01 9.4489000e-01 -8.0627000e-02 /
CHEB / 5.7966000e-01 4.7962000e-01 2.6567000e-02 /
CHEB / -1.0755000e-01 9.3512000e-02 7.3706000e-02 /
CHEB / -8.3553000e-02 -6.6906000e-02 4.8525000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H7O-13          -2.41 80.44 22.13 27.78 32.68 36.83 43.32 48.0
      53.09 null
```

```
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+C4H6-13(+m)=CO+C4H7O-13(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4456 (C5H7O2J(1447))    deltaHrxn(T=298K) = -
16.60852472958972 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1630000e+00 -6.1105000e-01 -2.3491000e-01 /
CHEB / 1.3710000e+01 5.9416000e-01 1.9737000e-01 /
CHEB / -4.2166000e-02 1.3648000e-01 8.0983000e-02 /
CHEB / -2.0267000e-01 -5.3937000e-02 -1.2430000e-03 /
CHEB / -1.3361000e-01 -5.8199000e-02 -2.7686000e-02 /

sSPC(2810)+C4H6-13(+m)=CO2+C4H7-24(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4456 (C5H7O2J(1447))    deltaHrxn(T=298K) = -
48.9450924342967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1763000e+00 -9.4916000e-01 -1.8283000e-01 /
CHEB / 9.9947000e+00 9.0396000e-01 9.8308000e-02 /
CHEB / -1.1228000e-01 2.1373000e-01 1.1256000e-01 /
CHEB / -2.8635000e-01 -5.8221000e-02 3.0389000e-02 /
CHEB / -1.8870000e-01 -8.2567000e-02 -2.5316000e-02 /

CO+C4H7O-13(+m)=CO2+C4H7-24(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4456 (C5H7O2J(1447))   deltaHrxn(T=298K) = -
32.336567704706965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6269000e+01 -6.1235000e-01 -2.1726000e-01 /
CHEB / 2.1744000e+01 6.2447000e-01 1.8690000e-01 /
CHEB / 6.4959000e-01 9.9978000e-02 7.2001000e-02 /
CHEB / 1.8979000e-02 -6.3127000e-02 -8.0826000e-03 /
CHEB / -3.8071000e-02 -5.1179000e-02 -2.6420000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!Here are the path reactions and their high-P limit kinetics:

HCO+C4H6O(717)(+m)=CO+CH3C[OH]CHcH2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5022 (C5H7O2J(1451))    deltaHrxn(T=298K) = -
16.998470470712704 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1875000e+01 2.4317000e-08 1.6927000e-08 /
CHEB / 1.9750000e+01 4.5839000e-08 3.1907000e-08 /
CHEB / 3.0293000e-01 3.9018000e-08 2.7159000e-08 /
CHEB / 1.0805000e-01 3.0439000e-08 2.1188000e-08 /
CHEB / 4.3350000e-02 2.1954000e-08 1.5281000e-08 /

HCO+C4H6O(717)(+m)=CO2+C4H7-24(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5022 (C5H7O2J(1451))   deltaHrxn(T=298K) = -
41.16565482281098 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1745000e+00 1.1615000e-08 7.8843000e-09 /
CHEB / 1.1852000e+01 2.6275000e-08 1.8542000e-08 /
CHEB / 2.7871000e-01 2.1270000e-08 1.4799000e-08 /
CHEB / 1.0012000e-01 1.6577000e-08 1.1466000e-08 /
CHEB / 4.0616000e-02 1.2743000e-08 8.8862000e-09 /

CO+CH3C[OH]CHcH2(+m)=CO2+C4H7-24(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5022 (C5H7O2J(1451))    deltaHrxn(T=298K) = -
24.167184352098275 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4455000e+01 -1.8525000e-04 -1.2894000e-04 /
CHEB / 2.7906000e+01 1.5022000e-04 1.0456000e-04 /
CHEB / 1.1014000e+00 5.6213000e-05 3.9126000e-05 /
CHEB / 3.7270000e-01 -1.0002000e-05 -6.9610000e-06 /
CHEB / 1.2082000e-01 -1.2955000e-05 -9.0170000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
```

```
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H6O(717)+HCO(+m)=CH3C[O]cHCH3+CO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5622 (C5H7O2J(1729))    deltaHrxn(T=298K) = -
17.19840005365014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2488000e+01 -3.2357000e-02 -2.1993000e-02 /
CHEB / 1.9753000e+01 3.1830000e-02 2.1525000e-02 /
CHEB / 4.2368000e-02 4.9459000e-03 3.4405000e-03 /
CHEB / -4.7573000e-02 -4.2605000e-03 -2.8451000e-03 /
CHEB / -4.8367000e-02 -2.2177000e-03 -1.5297000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+sC4H8O(+m)=CO2+CH3CH[OH]CH2CH2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6131 (C5H9O3J(874))
      deltaHrxn(T=298K) = -37.92629946024695 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9923000e+00 -5.9270000e-01 -2.3311000e-01 /
CHEB / 1.3619000e+01 5.1400000e-01 1.6294000e-01 /
CHEB / 9.4500000e-02 1.2245000e-01 6.5293000e-02 /
```

```
CHEB / -8.5053000e-02 -4.6468000e-02 1.0722000e-03 /
CHEB / -7.4403000e-02 -3.6753000e-02 -1.3883000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H9O2J(54) -59.88      99.03 28.58 34.95 40.59 45.37 53.3  58.61
      65.35 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+sC4H8O(+m)=CO+C4H9O2J(54)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6440 (C5H9O3J(1079))    deltaHrxn(T=298K) = -
8.749501594064242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7966000e+00 -3.6408000e-01 -1.7887000e-01 /
CHEB / 1.5949000e+01 3.5864000e-01 1.5693000e-01 /
CHEB / 1.7766000e-01 1.5659000e-02 2.1680000e-02 /
CHEB / 2.7781000e-02 -3.7379000e-02 -1.4876000e-02 /
CHEB / 1.3770000e-02 -5.5430000e-03 -5.8174000e-03 /

sSPC(2810)+sC4H8O(+m)=CO2+CH3CH[OH]CHCH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6440 (C5H9O3J(1079))
      deltaHrxn(T=298K) = -40.57595781233735 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.6417000e+00 -5.6506000e-01 -2.1628000e-01 /
CHEB / 1.2544000e+01 5.5486000e-01 1.7010000e-01 /
CHEB / 1.4561000e-02 4.0586000e-02 4.7340000e-02 /
CHEB / -4.3606000e-02 -5.4186000e-02 -1.1935000e-02 /
CHEB / -1.1586000e-02 -1.4859000e-02 -1.1868000e-02 /

CO+C4H9O2J(54)(+m)=CO2+CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6440 (C5H9O3J(1079))    deltaHrxn(T=298K) = -
31.82645621827311 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -1.7721000e+01 -2.9561000e-01 -1.5184000e-01 /
CHEB / 2.2160000e+01 3.2450000e-01 1.5265000e-01 /
CHEB / 1.1373000e+00 -1.6861000e-02 4.4794000e-03 /
CHEB / 3.2028000e-01 -3.8249000e-02 -1.9677000e-02 /
CHEB / 9.6514000e-02 -2.7617000e-04 -3.0693000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+MEKenol(+m)=CO2+CH3CH[OH]CHCH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #6756 (C5H9O3J(1078))
      deltaHrxn(T=298K) = -33.146609897531135 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0648000e+00 -2.8188000e-01 -1.6134000e-01 /
CHEB / 1.5044000e+01 2.9659000e-01 1.6318000e-01 /
CHEB / -5.4929000e-03 5.4071000e-02 3.7246000e-02 /
CHEB / -1.6388000e-01 -4.8513000e-02 -2.3422000e-02 /
CHEB / -1.4369000e-01 -3.6326000e-02 -2.2721000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
```

```
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3C[OH]cH  20.29 74.01 18.99 22.51 25.41 27.9  32.13 35.23 39.84
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+CH3C[OH]CHcH2(+m)=CO2+MEKenol(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #7049 (C5H8O3(2014))
      deltaHrxn(T=298K) = -91.84070183733452 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0444000e+01 -1.4284000e+00 -5.1929000e-02 /
CHEB / 2.0172000e+00 9.6123000e-01 -5.7991000e-02 /
CHEB / 3.4183000e-01 5.4958000e-01 2.6950000e-02 /
CHEB / -1.6122000e-01 1.5731000e-01 7.0433000e-02 /
CHEB / -1.6367000e-01 -6.3952000e-02 5.1038000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:
```

```
sSPC(2810)+CH3C[OH]CHcH2(+m)=CO2+sC4H8O(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #7466 (C5H8O3(1877))
      deltaHrxn(T=298K) = -84.4113539225283 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3792000e+00 -1.4789000e+00 -5.4624000e-02 /
CHEB / 2.6514000e+00 8.8558000e-01 -7.1870000e-02 /
CHEB / 3.3263000e-01 5.2279000e-01 3.2865000e-03 /
CHEB / -2.7492000e-01 1.6902000e-01 5.1459000e-02 /
CHEB / -2.4571000e-01 -3.2878000e-02 4.7815000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!Here are the path reactions and their high-P limit kinetics:

CO+sSPC(1697)(+m)=CO2+CH3O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7827 (C2H3O3J(850))    deltaHrxn(T=298K) = -
67.75278200646373 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6443000e+00 -2.4023000e-08 -1.6722000e-08 /
CHEB / 7.3015000e-01 -4.7120000e-08 -3.2799000e-08 /
CHEB / -6.3112000e-03 -4.4378000e-08 -3.0891000e-08 /
CHEB / 1.4224000e-03 -3.9930000e-08 -2.7794000e-08 /
CHEB / -4.5407000e-03 -3.3948000e-08 -2.3630000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+CH2O(+m)=CO2+CH3O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8025 (C2H3O3J(894))    deltaHrxn(T=298K) = -
25.627285280282496 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.7137000e+00 -1.5389000e-03 -1.0704000e-03 /
CHEB / 1.7304000e+01 -1.0043000e-04 -6.9705000e-05 /
CHEB / 2.2127000e-01 5.1496000e-04 3.5797000e-04 /
CHEB / 5.9600000e-02 1.6887000e-04 1.1736000e-04 /
CHEB / 6.4083000e-03 -7.9495000e-05 -5.5211000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H5O-3           -4.24 65.64 14.5  17.89 20.91 23.56 27.77 30.91
      33.76 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+CH3CO=sSPC(1590)   5.2000000e+11      0.00000
6.5600000e+03
!     C2H5O-3+CO=sSPC(1590)   5.3800000e+02      3.29000
1.0450000e+05
!     O+CH2C[O]CH3=sSPC(1590) 1.0000000e+13      0.00000
0.0000000e+00

sSPC(1590)(+m)=CH2O+CH3CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590))   deltaHrxn(T=298K) = 4.4689085819654
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 5.8510000e+00 1.9826000e+00 -1.0993000e-02 /
CHEB / 3.1955000e-01 -1.3706000e-02 -7.5658000e-03 /
CHEB / -1.7745000e+00 -2.5412000e-03 -4.2128000e-04 /
CHEB / -8.1428000e-01 5.2549000e-04 1.1306000e-03 /
CHEB / -3.5320000e-01 7.0286000e-04 8.5943000e-04 /

sSPC(1590)(+m)=C2H5O-3+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590))   deltaHrxn(T=298K) = 2.039085123161019
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.8585000e+01 2.2100000e+00 1.3229000e-01 /
CHEB / 3.5008000e+01 2.3710000e-01 1.4181000e-01 /
CHEB / -1.1778000e+00 1.1240000e-01 6.2518000e-02 /
CHEB / -5.9979000e-01 5.1636000e-02 2.6621000e-02 /
CHEB / -2.6933000e-01 2.4348000e-02 1.1877000e-02 /

C2H5O-3+CO(+m)=CH2O+CH3CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590))   deltaHrxn(T=298K) = 2.429823458804381
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0842000e+01 6.7416000e-08 4.6927000e-08 /
CHEB / 3.6873000e+01 1.2718000e-07 8.8529000e-08 /
CHEB / 4.0745000e-01 1.0804000e-07 7.5205000e-08 /
CHEB / 1.8485000e-01 8.3327000e-08 5.8002000e-08 /
CHEB / 8.2737000e-02 5.8604000e-08 4.0793000e-08 /

O+CH2C[O]CH3(+m)=sSPC(1590)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Oa     C_rad/H2/CO       deltaHrxn(T=298K) = -
89.3302062665808 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0130000e+01 2.2077000e+00 1.3071000e-01 /
CHEB / -2.0976000e+00 2.3383000e-01 1.3953000e-01 /
CHEB / -1.3636000e+00 1.1032000e-01 6.1072000e-02 /
CHEB / -6.4710000e-01 5.0384000e-02 2.5751000e-02 /
CHEB / -2.9333000e-01 2.3617000e-02 1.1369000e-02 /

O+CH2C[O]CH3(+m)=CH2O+CH3CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590))   deltaHrxn(T=298K) = -84.86129768461541
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3093000e+01 3.9106000e-08 2.7221000e-08 /
CHEB / -8.9951000e-02 7.5254000e-08 5.2382000e-08 /
CHEB / -2.3035000e-02 6.7153000e-08 4.6743000e-08 /
CHEB / 1.3467000e-03 5.5688000e-08 3.8763000e-08 /
CHEB / -1.0873000e-02 4.2885000e-08 2.9851000e-08 /

O+CH2C[O]CH3(+m)=C2H5O-3+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(1590))   deltaHrxn(T=298K) = -87.29112114341979
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / -1.7508000e+00 -4.6598000e-06 -3.2436000e-06 /
CHEB / 9.6072000e+00 3.6893000e-07 2.5681000e-07 /
CHEB / 1.3271000e+00 2.0501000e-06 1.4270000e-06 /
CHEB / 4.3676000e-01 9.6474000e-07 6.7153000e-07 /
CHEB / 1.1575000e-01 2.4149000e-07 1.6809000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sC4H8O+HCO(+m)=C2H5O-2+C3H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #33 (C5H9O2J(401))      deltaHrxn(T=298K) = -
4.3796594606292025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0522000e+00 -5.5485000e-01 -1.4439000e-01 /
CHEB / 3.1063000e+00 7.1419000e-01 1.5700000e-01 /
CHEB / -9.5688000e-02 -8.1157000e-02 2.9177000e-02 /
CHEB / -3.5862000e-02 -9.5407000e-02 -3.7330000e-02 /
CHEB / 2.2102000e-02 -1.1175000e-02 -1.8938000e-02 /

C2H5O-2+C3H4O(+m)=CH3CH[OH]CH2CH2+CO(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #33 (C5H9O2J(401)) deltaHrxn(T=298K) = -
14.618523760866637 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2707000e+01 -2.1383000e-04 -1.4951000e-04 /
CHEB / 2.0421000e+01 2.0463000e-04 1.4314000e-04 /
CHEB / 3.2016000e-01 5.2299000e-05 3.6551000e-05 /
CHEB / 1.4125000e-01 -2.7631000e-05 -1.9409000e-05 /
CHEB / 6.3551000e-02 -1.7895000e-05 -1.2512000e-05 /
```

```
sC4H8O+HCO(+m)=CH3CH[OH]CH2CH2+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #33 (C5H9O2J(401)) deltaHrxn(T=298K) = -
18.998183221495836 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0352000e+01 5.1135000e-05 3.5726000e-05 /
CHEB / 1.8777000e+01 -4.2442000e-05 -2.9672000e-05 /
CHEB / 2.6284000e-01 -1.7772000e-05 -1.2411000e-05 /
CHEB / 1.1256000e-01 4.2904000e-06 3.0160000e-06 /
CHEB / 5.0442000e-02 5.0954000e-06 3.5624000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sC4H8O+HCO(+m)=CH3CH[OH]CHCH3+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #59 (C5H9O2J(402)) deltaHrxn(T=298K) = -
21.647841573586234 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9970000e+00 -7.2734000e-02 -4.8203000e-02 /
CHEB / 1.7708000e+01 5.1312000e-02 3.3162000e-02 /
CHEB / 1.8707000e-01 -2.8819000e-03 -1.5991000e-03 /
CHEB / 6.3111000e-02 -8.8465000e-03 -5.7357000e-03 /
CHEB / 2.6805000e-02 4.9704000e-04 2.0902000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
```

```
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

HCO+MEKenol(+m)=CO+CH3CH[OH]CHCH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #92 (C5H9O2J(499)) deltaHrxn(T=298K) = -
14.21849365878002 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1951000e+01 5.6551000e-07 3.9366000e-07 /
CHEB / 2.0455000e+01 3.6304000e-07 2.5271000e-07 /
CHEB / 2.4890000e-01 -1.6356000e-07 -1.1388000e-07 /
CHEB / 8.9374000e-02 -2.0899000e-07 -1.4549000e-07 /
CHEB / 2.2209000e-02 -9.1017000e-08 -6.3354000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!Here are the path reactions and their high-P limit kinetics:

CO+sSPC(2810)(+m)=CO2+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #172 (C2HO3J(351))      deltaHrxn(T=298K) = -
18.928116238751116 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1517000e+00 -5.2205000e-09 -3.6339000e-09 /
CHEB / 2.5999000e+00 -8.9231000e-09 -6.2111000e-09 /
CHEB / -3.1007000e-01 -5.1193000e-09 -3.5634000e-09 /
CHEB / -5.9394000e-02 -7.8069000e-10 -5.4342000e-10 /
CHEB / 7.9917000e-03 2.4214000e-09 1.6855000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O2             -32.6 55.66 10.42 11.44 12.34 13.32 14.3  15.22
      16.86 null
!Here are the path reactions and their high-P limit kinetics:
!     OCOOH+H=sSPC(3121)      1.4157154e+13      -0.15000
2.9166667e+02
!     HCO+HO2=sSPC(3121)      1.4157154e+13      -0.15000
2.9166667e+02
!     sSPC(2810)+OH=sSPC(3121)      2.0000000e+13      0.00000
0.0000000e+00
!     sSPC(3071)+H=sSPC(3121) 1.4157154e+13      -0.15000
2.9166667e+02
!     CO+H2O2=sSPC(3121)      1.2700000e-01      3.70000
5.3360000e+04

OCOOH+H(+m)=sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
95.87955775036043 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0688000e+01 3.1684000e+00 5.1713000e-01 /
CHEB / -1.0314000e+00 6.7954000e-01 1.9254000e-01 /
CHEB / -6.3362000e-01 2.2804000e-01 4.4863000e-02 /
CHEB / -2.3557000e-01 8.7770000e-02 1.3771000e-02 /
CHEB / -8.1010000e-02 3.5406000e-02 4.5840000e-03 /

HCO+HO2(+m)=sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) High-P Limit: R_Recombination estimate:
(Average:) CO_pri_rad     O_rad/NonDe           deltaHrxn(T=298K) = -
82.44146738912778 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6074000e+00 3.1618000e+00 5.1253000e-01 /
CHEB / -1.0377000e+00 6.7066000e-01 1.8637000e-01 /
CHEB / -6.7276000e-01 2.2271000e-01 4.1162000e-02 /
CHEB / -3.0409000e-01 8.4680000e-02 1.1632000e-02 /
CHEB / -1.2619000e-01 3.3657000e-02 3.3739000e-03 /
```

```
OCOOH+H(+m)=HCO+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#206 (sSPC(3121)) deltaHrxn(T=298K) = -13.438090361232659 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0548000e+01 -1.1551000e-05 -8.0405000e-06 /
CHEB / 2.6303000e-01 2.1537000e-06 1.4991000e-06 /
CHEB / 3.2826000e-01 4.9513000e-06 3.4465000e-06 /
CHEB / 1.8968000e-01 1.7677000e-06 1.2304000e-06 /
CHEB / 8.4598000e-02 1.3002000e-07 9.0507000e-08 /

sSPC(2810)+OH(+m)=sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     O_pri_rad      deltaHrxn(T=298K) = -
42.6354887777726 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1417000e+01 1.7831000e+00 -1.1882000e-01 /
CHEB / -1.7259000e+00 4.7366000e-02 4.3481000e-02 /
CHEB / -8.1950000e-01 7.0588000e-02 4.0555000e-02 /
CHEB / -3.5671000e-01 2.7581000e-02 1.2510000e-02 /
CHEB / -1.4633000e-01 5.0884000e-03 9.8680000e-04 /

OCOOH+H(+m)=sSPC(2810)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -53.24406897258783
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3162000e+01 3.4632000e-08 2.4106000e-08 /
CHEB / -3.2257000e-01 3.4602000e-08 2.4086000e-08 /
CHEB / 1.7213000e-02 1.4925000e-08 1.0389000e-08 /
CHEB / 8.1391000e-02 4.7487000e-09 3.3055000e-09 /
CHEB / 5.0529000e-02 5.7245000e-10 3.9850000e-10 /

HCO+HO2(+m)=sSPC(2810)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -39.80597861135517
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3055000e+01 1.3605000e-08 9.4701000e-09 /
CHEB / -3.1426000e-01 2.3306000e-08 1.6223000e-08 /
CHEB / -1.4333000e-02 1.6005000e-08 1.1141000e-08 /
CHEB / 1.6485000e-02 8.9112000e-09 6.2029000e-09 /
CHEB / 7.0431000e-03 4.0232000e-09 2.8005000e-09 /

sSPC(3071)+H(+m)=sSPC(3121)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
95.21996406589759 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0920000e+01 3.1684000e+00 5.1713000e-01 /
CHEB / -8.8646000e-01 6.7954000e-01 1.9254000e-01 /
CHEB / -6.5252000e-01 2.2804000e-01 4.4863000e-02 /
CHEB / -2.7156000e-01 8.7770000e-02 1.3771000e-02 /
CHEB / -1.0542000e-01 3.5406000e-02 4.5840000e-03 /
```

```
sSPC(3071)+H(+m)=OCOOH+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = 0.6595936844628554
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1889000e+00 -1.7599000e-05 -1.2250000e-05 /
CHEB / 8.9577000e-01 9.7241000e-06 6.7686000e-06 /
CHEB / 3.9329000e-01 4.5478000e-06 3.1655000e-06 /
CHEB / 9.2823000e-02 7.1276000e-07 4.9615000e-07 /
CHEB / 4.0718000e-02 2.2359000e-07 1.5564000e-07 /

sSPC(3071)+H(+m)=HCO+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -12.778496676769807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0316000e+01 -1.1551000e-05 -8.0405000e-06 /
CHEB / 4.0798000e-01 2.1537000e-06 1.4991000e-06 /
CHEB / 3.0936000e-01 4.9513000e-06 3.4465000e-06 /
CHEB / 1.5369000e-01 1.7677000e-06 1.2304000e-06 /
CHEB / 6.0191000e-02 1.3002000e-07 9.0507000e-08 /

sSPC(3071)+H(+m)=sSPC(2810)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -52.584475288124985
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2930000e+01 3.4632000e-08 2.4106000e-08 /
CHEB / -1.7762000e-01 3.4602000e-08 2.4086000e-08 /
CHEB / -1.6821000e-03 1.4925000e-08 1.0389000e-08 /
CHEB / 4.5399000e-02 4.7487000e-09 3.3055000e-09 /
CHEB / 2.6121000e-02 5.7245000e-10 3.9850000e-10 /

CO+H2O2(+m)=sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) High-P Limit: 1,2_Insertion exact:  RO_H
CO_birad          deltaHrxn(T=298K) = -12.598422041612828 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4930000e+01 3.1363000e+00 4.9490000e-01 /
CHEB / 1.8965000e+01 6.3706000e-01 1.6325000e-01 /
CHEB / -2.2166000e-01 2.0298000e-01 2.7643000e-02 /
CHEB / -1.3760000e-01 7.3528000e-02 4.0268000e-03 /
CHEB / -5.7232000e-02 2.7484000e-02 -8.1291000e-04 /

OCOOH+H(+m)=CO+H2O2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#206 (sSPC(3121)) deltaHrxn(T=298K) = -83.2811357087476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6995000e+00 -5.8849000e-06 -4.0963000e-06 /
CHEB / 1.6566000e+00 -1.6292000e-07 -1.1341000e-07 /
CHEB / 6.1449000e-01 2.2774000e-06 1.5853000e-06 /
CHEB / 2.9940000e-01 1.2520000e-06 8.7147000e-07 /
CHEB / 1.3542000e-01 3.4621000e-07 2.4099000e-07 /

HCO+HO2(+m)=CO+H2O2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#206 (sSPC(3121)) deltaHrxn(T=298K) = -69.84304534751494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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```
CHEB / 5    3 /
CHEB / 7.1057000e+00 -2.0732000e-05 -1.4431000e-05 /
CHEB / 1.8900000e+00 5.2065000e-06 3.6242000e-06 /
CHEB / 6.7388000e-01 9.6287000e-06 6.7023000e-06 /
CHEB / 2.5716000e-01 3.0659000e-06 2.1341000e-06 /
CHEB / 9.5369000e-02 -1.0887000e-07 -7.5789000e-08 /

sSPC(2810)+OH(+m)=CO+H2O2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -30.037066736159773
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1487000e-01 4.2152000e-09 2.9146000e-09 /
CHEB / 9.5128000e+00 8.2738000e-09 5.7551000e-09 /
CHEB / 4.5077000e-01 7.2946000e-09 5.0936000e-09 /
CHEB / 1.8531000e-01 5.7099000e-09 3.9845000e-09 /
CHEB / 7.8105000e-02 4.0183000e-09 2.7975000e-09 /

sSPC(3071)+H(+m)=CO+H2O2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #206 (sSPC(3121)) deltaHrxn(T=298K) = -82.62154202428476
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4674000e+00 -5.8849000e-06 -4.0963000e-06 /
CHEB / 1.8016000e+00 -1.6292000e-07 -1.1341000e-07 /
CHEB / 5.9559000e-01 2.2774000e-06 1.5853000e-06 /
CHEB / 2.6341000e-01 1.2520000e-06 8.7147000e-07 /
CHEB / 1.1102000e-01 3.4621000e-07 2.4099000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCOOH       -90.2 59.4  10.83 12.87 14.62 15.98 18.4  20.0  20.0
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     H2                0.0   -1.38 0.0   0.0   0.0   0.0   0.0   0.0
      0.0   null
!Here are the path reactions and their high-P limit kinetics:
!     HCO+OH=HCOOH            1.4157154e+13      -0.15000
2.9166667e+02
```

```
!     sSPC(2810)+H=HCOOH      1.4157154e+13      -0.15000
2.9166667e+02
!     CO+H2O=HCOOH            1.2700000e-01      3.70000
5.3360000e+04
!     CO2+H2=HCOOH            1.5100000e+09      1.23000
7.3900000e+04

sSPC(2810)+H(+m)=HCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (HCOOH) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     H_rad          deltaHrxn(T=298K) = -
100.8892812158762 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9220000e+00 7.6881000e+00 -1.9286000e-01 /
CHEB / -6.0630000e+00 -6.3857000e-01 1.8094000e+00 /
CHEB / -2.0193000e+00 -1.3975000e+00 2.1638000e-03 /
CHEB / -6.9824000e-01 -6.1334000e-01 -2.6499000e-01 /
CHEB / -2.3283000e-01 -1.8073000e-01 -1.3414000e-01 /

sSPC(2810)+H(+m)=HCO+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (HCOOH)      deltaHrxn(T=298K) = 9.018936335357411
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0728000e+01 -8.1290000e-02 -6.6590000e-02 /
CHEB / 1.6629000e+00 9.1161000e-02 7.9023000e-02 /
CHEB / -1.5491000e-01 6.5779000e-03 -1.9524000e-03 /
CHEB / 4.0615000e-02 -1.5451000e-02 -1.0416000e-02 /
CHEB / 4.4760000e-02 -4.7980000e-03 -2.5343000e-03 /

HCO+OH(+m)=CO+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#237 (HCOOH)      deltaHrxn(T=298K) = -103.92947016591695 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2618000e+01 6.2995000e-02 -7.4542000e-03 /
CHEB / 4.6403000e-02 -7.8761000e-02 2.1056000e-02 /
CHEB / -1.0917000e-01 8.2481000e-03 -1.9653000e-02 /
CHEB / 1.6277000e-02 8.2750000e-03 2.6695000e-03 /
CHEB / 2.8597000e-02 1.0262000e-03 4.7510000e-03 /

sSPC(2810)+H(+m)=CO+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (HCOOH)      deltaHrxn(T=298K) = -94.91053383055954
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2736000e+01 -1.3627000e-01 -9.2633000e-02 /
CHEB / -3.7094000e-02 1.9798000e-01 1.3006000e-01 /
CHEB / -5.9646000e-02 -6.0258000e-02 -3.1200000e-02 /
CHEB / 3.7393000e-02 -1.0613000e-02 -1.3595000e-02 /
CHEB / 3.6135000e-02 7.2767000e-03 4.8102000e-03 /

HCO+OH(+m)=CO2+H2(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#237 (HCOOH)      deltaHrxn(T=298K) = -113.75746675733585 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8906000e+00 3.2030000e-02 -2.1856000e-02 /
CHEB / -2.0561000e+00 -4.2338000e-02 3.5407000e-02 /
```

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CHEB / -6.4465000e-01 7.8264000e-03 -1.5695000e-02 /
CHEB / -1.6547000e-01 3.2867000e-03 -4.8769000e-04 /
CHEB / -4.0541000e-02 -2.0326000e-04 2.9985000e-03 /

sSPC(2810)+H(+m)=CO2+H2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (HCOOH)      deltaHrxn(T=298K) = -104.73853042197844
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9408000e+00 -1.7382000e-01 -1.0793000e-01 /
CHEB / -2.1158000e+00 2.3983000e-01 1.4342000e-01 /
CHEB / -5.8491000e-01 -5.7793000e-02 -2.4881000e-02 /
CHEB / -1.4217000e-01 -1.6381000e-02 -1.6208000e-02 /
CHEB / -3.2936000e-02 4.9602000e-03 2.2692000e-03 /

CO2+H2(+m)=CO+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#237 (HCOOH)      deltaHrxn(T=298K) = 9.827996591418888 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7915000e+01 -7.3678000e-01 -2.2256000e-01 /
CHEB / 2.5923000e+01 7.8899000e-01 1.6924000e-01 /
CHEB / 1.4547000e-01 6.3331000e-02 1.0296000e-01 /
CHEB / 2.3333000e-02 -7.2189000e-02 -1.1421000e-02 /
CHEB / -3.5537000e-04 -4.8553000e-02 -3.2055000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     C3H5OJ(12)        -1.58 70.39 18.06 21.84 25.19 28.08 32.66 36.06
      41.31 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3CHCHCHO  -28.19      75.98 22.26 27.43 31.78 35.41 41.16 45.23
      50.19 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:
```

```
C2H5O-2+C3H5OJ(12)(+m)=CH3CH[OH]CHCH3+HCO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C5H10O2(332))
      deltaHrxn(T=298K) = 0.8099440021388986 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6532000e+00 -1.3514000e+00 -4.9301000e-02 /
CHEB / 3.5776000e+00 1.0469000e+00 -4.5049000e-02 /
CHEB / 2.4008000e-01 5.0368000e-01 4.6490000e-02 /
CHEB / -3.1067000e-01 4.5506000e-02 7.5025000e-02 /
CHEB / -2.0146000e-01 -1.3886000e-01 3.1403000e-02 /

C2H5O-2+C3H5OJ(12)(+m)=sBuOH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C5H10O2(332))     deltaHrxn(T=298K) = -
82.35167100384948 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2241000e+00 -1.3514000e+00 -4.9301000e-02 /
CHEB / 4.7812000e+00 1.0469000e+00 -4.5049000e-02 /
CHEB / 5.5640000e-01 5.0368000e-01 4.6490000e-02 /
CHEB / -1.9985000e-01 4.5506000e-02 7.5025000e-02 /
CHEB / -1.5784000e-01 -1.3886000e-01 3.1403000e-02 /

CH3CH[OH]CHCH3+HCO(+m)=sBuOH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C5H10O2(332))     deltaHrxn(T=298K) = -
83.16161500598837 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8256000e+00 -1.3514000e+00 -4.9301000e-02 /
CHEB / 4.6969000e+00 1.0469000e+00 -4.5049000e-02 /
CHEB / 6.2312000e-01 5.0368000e-01 4.6490000e-02 /
CHEB / -1.7794000e-01 4.5506000e-02 7.5025000e-02 /
CHEB / -1.4907000e-01 -1.3886000e-01 3.1403000e-02 /

C2H5O-2+C3H5OJ(12)(+m)=CH3CHCHCHO+CH3OH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C5H10O2(332))
      deltaHrxn(T=298K) = -61.69356340051404 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5921000e+00 -1.3988000e+00 -4.2713000e-02 /
CHEB / 2.6312000e+00 1.0050000e+00 -4.4876000e-02 /
CHEB / 3.4718000e-01 5.5118000e-01 3.1765000e-02 /
CHEB / -2.5424000e-01 1.1833000e-01 6.8384000e-02 /
CHEB / -2.1376000e-01 -1.1132000e-01 4.1452000e-02 /

CH3CH[OH]CHCH3+HCO(+m)=CH3CHCHCHO+CH3OH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #270 (C5H10O2(332))
      deltaHrxn(T=298K) = -62.50350740265294 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1936000e+00 -1.3988000e+00 -4.2713000e-02 /
CHEB / 2.5469000e+00 1.0050000e+00 -4.4876000e-02 /
CHEB / 4.1391000e-01 5.5118000e-01 3.1765000e-02 /
CHEB / -2.3233000e-01 1.1833000e-01 6.8384000e-02 /
CHEB / -2.0499000e-01 -1.1132000e-01 4.1452000e-02 /
```

```
CH3CHCHCHO+CH3OH(+m)=sBuOH+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #270 (C5H10O2(332))     deltaHrxn(T=298K) = -
20.658107603335424 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8149000e+01 -1.3988000e+00 -4.2713000e-02 /
CHEB / 2.5004000e+01 1.0050000e+00 -4.4876000e-02 /
CHEB / 6.9354000e-01 5.5118000e-01 3.1765000e-02 /
CHEB / -1.5278000e-01 1.1833000e-01 6.8384000e-02 /
CHEB / -1.8033000e-01 -1.1132000e-01 4.1452000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H5OJ(13)        4.5   76.14 18.65 22.05 25.01 27.57 32.16 35.43
      39.19 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sBuOH       -70.43      83.94 26.98 33.77 39.97 44.89 52.94 58.89
      68.36 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

HCO+CH3CH[OH]CH2CH2(+m)=C3H5OJ(13)+C2H5O-2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #305 (C5H10O2(349))
      deltaHrxn(T=298K) = 2.6196179104872233 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8320000e+00 -1.3330000e+00 -5.0597000e-02 /
CHEB / 2.9057000e+00 1.0498000e+00 -4.0871000e-02 /
CHEB / 1.0114000e-01 4.6915000e-01 4.9890000e-02 /
CHEB / -2.7383000e-01 2.7305000e-02 6.5028000e-02 /
CHEB / -1.5470000e-01 -1.2319000e-01 1.9833000e-02 /
```

```
CH2CHO+CH3CH[OH]CH2(+m)=HCO+CH3CH[OH]CH2CH2(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #305 (C5H10O2(349))
      deltaHrxn(T=298K) = -0.8201788981641904 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0405000e+01 -1.3478000e+00 -4.8012000e-02 /
CHEB / 2.7656000e+00 1.0395000e+00 -4.1663000e-02 /
CHEB / 2.0598000e-01 4.8458000e-01 4.4593000e-02 /
CHEB / -2.8032000e-01 4.4261000e-02 6.4045000e-02 /
CHEB / -1.7612000e-01 -1.1946000e-01 2.3295000e-02 /

CH2CHO+CH3CH[OH]CH2(+m)=C3H5OJ(13)+C2H5O-2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #305 (C5H10O2(349))
      deltaHrxn(T=298K) = 1.7994390123230328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8378000e+00 -1.3330000e+00 -5.0597000e-02 /
CHEB / 2.6863000e+00 1.0498000e+00 -4.0871000e-02 /
CHEB / 7.3664000e-02 4.6915000e-01 4.9890000e-02 /
CHEB / -3.1055000e-01 2.7305000e-02 6.5028000e-02 /
CHEB / -1.8265000e-01 -1.2319000e-01 1.9833000e-02 /

HCO+CH3CH[OH]CH2CH2(+m)=CO+sBuOH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #305 (C5H10O2(349))      deltaHrxn(T=298K) = -
85.81127335807876 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0572000e+00 -1.3478000e+00 -4.8012000e-02 /
CHEB / 4.1446000e+00 1.0395000e+00 -4.1663000e-02 /
CHEB / 5.3823000e-01 4.8458000e-01 4.4593000e-02 /
CHEB / -1.3683000e-01 4.4261000e-02 6.4045000e-02 /
CHEB / -1.0614000e-01 -1.1946000e-01 2.3295000e-02 /

C3H5OJ(13)+C2H5O-2(+m)=CO+sBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #305 (C5H10O2(349))     deltaHrxn(T=298K) = -
88.43089126856599 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9327000e+00 -1.3330000e+00 -5.0597000e-02 /
CHEB / 3.2546000e+00 1.0498000e+00 -4.0871000e-02 /
CHEB / 4.6824000e-01 4.6915000e-01 4.9890000e-02 /
CHEB / -1.2833000e-01 2.7305000e-02 6.5028000e-02 /
CHEB / -9.0937000e-02 -1.2319000e-01 1.9833000e-02 /

CH2CHO+CH3CH[OH]CH2(+m)=CO+sBuOH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #305 (C5H10O2(349))      deltaHrxn(T=298K) = -
86.63145225624295 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0630000e+00 -1.3478000e+00 -4.8012000e-02 /
CHEB / 3.9252000e+00 1.0395000e+00 -4.1663000e-02 /
CHEB / 5.1075000e-01 4.8458000e-01 4.4593000e-02 /
CHEB / -1.7354000e-01 4.4261000e-02 6.4045000e-02 /
CHEB / -1.3409000e-01 -1.1946000e-01 2.3295000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH3CH[OH]CHCH3    -24.08      88.38 25.48 31.44 36.87 41.5  49.19
      54.44 63.16 null
!     sSPC(116)   -58.3 100.11      33.34 40.65 47.04 51.68 59.43 65.39
      74.77 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(116)+HCO(+m)=sSPC(3071)+CH3CH[OH]CHCH3(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #466 (C5H10O4(353))
      deltaHrxn(T=298K) = -1.5694702506267895 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1755000e+00 -5.3508000e-02 -3.5734000e-02 /
CHEB / 4.4098000e+00 3.2102000e-02 2.1110000e-02 /
CHEB / 1.0656000e+00 -6.4104000e-03 -4.1812000e-03 /
CHEB / 1.9692000e-01 -1.4893000e-02 -9.7438000e-03 /
CHEB / -3.0448000e-03 -3.8041000e-03 -2.5663000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-2           -12.91      68.02 16.13 19.18 21.77 24.02 27.63
      30.4  32.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
```

```
!     CH3CH[OH]CH2CH2   -21.43      87.36 26.21 32.41 38.06 42.49 49.78
      55.15 63.7  null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(332)   -53.93      102.11      32.84 39.97 46.09 50.94 58.78
      64.89 72.26 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(332)+HCO(+m)=CH3CH[OH]CH2CH2+sSPC(3071)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #517 (C5H10O4(749))
      deltaHrxn(T=298K) = -3.2893461631070444 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1612000e+00 -1.9106000e-02 -1.3066000e-02 /
CHEB / 4.0957000e+00 2.0711000e-02 1.4129000e-02 /
CHEB / 1.0845000e+00 2.1226000e-03 1.4792000e-03 /
CHEB / 2.2022000e-01 -3.4888000e-03 -2.3591000e-03 /
CHEB / 4.2069000e-03 -8.5536000e-04 -6.0038000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
sSPC(3071)+C4H7-24(+m)=CH3CH[o]C2H3+sSPC(2810)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #586 (C5H8O3(407))
      deltaHrxn(T=298K) = -33.07656998937506 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2993000e+01 -8.6894000e-02 -5.6441000e-02 /
CHEB / -3.2658000e-01 5.3167000e-02 3.4026000e-02 /
CHEB / -3.6890000e-02 1.3967000e-02 8.4215000e-03 /
CHEB / -2.7933000e-02 -1.6923000e-02 -1.0460000e-02 /
CHEB / -2.5076000e-02 -6.6544000e-03 -4.2543000e-03 /

sSPC(46)+HCO(+m)=CH3CH[o]C2H3+sSPC(2810)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #586 (C5H8O3(407))
      deltaHrxn(T=298K) = -49.03467988099477 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3282000e+01 -2.1264000e-02 -1.4576000e-02 /
CHEB / -5.2162000e-01 2.0493000e-04 2.3654000e-04 /
CHEB / -2.6514000e-02 -1.8754000e-04 -8.7399000e-05 /
CHEB / 1.0534000e-02 -5.7405000e-03 -3.8795000e-03 /
CHEB / -5.9950000e-04 -3.2204000e-03 -2.1697000e-03 /

sSPC(46)+HCO(+m)=sSPC(3071)+C4H7-24(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #586 (C5H8O3(407)) deltaHrxn(T=298K) = -
15.958109891619713 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7728000e+00 -1.4836000e-02 -1.0220000e-02 /
CHEB / 1.8802000e+00 3.2787000e-03 2.2774000e-03 /
CHEB / 7.5551000e-01 -1.1190000e-03 -7.5989000e-04 /
CHEB / 2.0466000e-01 -4.7986000e-03 -3.2774000e-03 /
CHEB / 3.7350000e-02 -2.2979000e-03 -1.5677000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     C4H7-24           32.88 70.64 20.08 25.18 29.64 33.46 39.5  43.98
      50.91 null
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!Here are the path reactions and their high-P limit kinetics:

sSPC(56)+HCO(+m)=sSPC(3071)+C4H7-24(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #711 (C5H8O3(460)) deltaHrxn(T=298K) = -
17.52793671822434 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2862000e+00 -8.9126000e-03 -6.1676000e-03 /
CHEB / 2.2943000e+00 2.2174000e-03 1.5380000e-03 /
CHEB / 7.8761000e-01 5.9647000e-04 4.1132000e-04 /
CHEB / 2.2976000e-01 -2.1226000e-03 -1.4620000e-03 /
CHEB / 4.3167000e-02 -9.6313000e-04 -6.6311000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     sSPC(752)   -43.28      96.95 29.5  36.01 41.56 45.92 52.92 58.39
      64.94 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(752)+HCO(+m)=sSPC(3071)+CH3C[O]cHCH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #842 (C5H8O4(597))
      deltaHrxn(T=298K) = -3.289488983712925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5002000e+00 -1.9832000e-02 -1.3552000e-02 /
CHEB / 3.3262000e+00 2.1258000e-02 1.4492000e-02 /
CHEB / 9.4297000e-01 2.4542000e-03 1.7049000e-03 /
CHEB / 1.7713000e-01 -3.5003000e-03 -2.3634000e-03 /
CHEB / -8.5325000e-03 -1.0272000e-03 -7.1638000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3071)+CH2C[O]CH3(+m)=sSPC(1590)+sSPC(2810)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #953 (C4H6O4(853))
      deltaHrxn(T=298K) = -42.695086553151974 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3384000e+01 -1.1080000e-04 -9.4302000e-05 /
CHEB / -6.4366000e-01 1.1876000e-05 9.7098000e-06 /
CHEB / -5.8303000e-02 1.5618000e-04 1.3221000e-04 /
CHEB / -1.5278000e-02 2.0787000e-05 1.7271000e-05 /
CHEB / -2.6190000e-02 -6.8079000e-05 -5.8016000e-05 /

sSPC(1356)+HCO(+m)=sSPC(1590)+sSPC(2810)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #953 (C4H6O4(853))
      deltaHrxn(T=298K) = -49.03467994325158 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3034000e+01 -1.5487000e-06 -1.5849000e-06 /
CHEB / -3.3304000e-01 2.1585000e-06 1.3261000e-06 /
CHEB / -4.3091000e-02 7.6325000e-06 6.0531000e-06 /
CHEB / -1.0330000e-03 4.8467000e-06 3.7832000e-06 /
CHEB / -1.1195000e-02 -1.4780000e-07 -3.6048000e-07 /

sSPC(1356)+HCO(+m)=sSPC(3071)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #953 (C4H6O4(853))
      deltaHrxn(T=298K) = -6.3395933900996075 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1533000e+00 -3.4047000e-03 -2.3642000e-03 /
CHEB / 2.9115000e+00 3.0183000e-03 2.0954000e-03 /
CHEB / 8.9877000e-01 1.0356000e-03 7.1877000e-04 /
CHEB / 2.0397000e-01 -4.3469000e-04 -3.0083000e-04 /
CHEB / 1.8327000e-02 -2.7856000e-04 -1.9325000e-04 /
```

```
sSPC(1590)+sSPC(2810)(+m)=sSPC(1474)+CO(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #953 (C4H6O4(853))
      deltaHrxn(T=298K) = -23.878079473713072 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3924000e+00 -2.2205000e-02 -1.7953000e-02 /
CHEB / 1.1229000e+01 2.0061000e-02 1.6408000e-02 /
CHEB / 5.4761000e-01 9.8572000e-03 7.6249000e-03 /
CHEB / 1.9634000e-01 -6.0744000e-03 -4.8209000e-03 /
CHEB / 7.3689000e-02 -3.2196000e-03 -2.4571000e-03 /

sSPC(3071)+CH2C[O]CH3(+m)=sSPC(1474)+CO(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #953 (C4H6O4(853))
      deltaHrxn(T=298K) = -66.57316602686504 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1849000e+00 -6.6569000e-03 -4.6223000e-03 /
CHEB / 3.4466000e+00 5.9127000e-03 4.1062000e-03 /
CHEB / 1.1523000e+00 2.2741000e-03 1.5762000e-03 /
CHEB / 3.3240000e-01 -1.0483000e-03 -7.2566000e-04 /
CHEB / 7.2843000e-02 -6.5322000e-04 -4.5245000e-04 /

sSPC(1356)+HCO(+m)=sSPC(1474)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #953 (C4H6O4(853)) deltaHrxn(T=298K) = -
72.91275941696466 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2740000e+00 -2.9658000e-03 -2.0640000e-03 /
CHEB / 3.4096000e+00 2.1899000e-03 1.5242000e-03 /
CHEB / 1.1103000e+00 1.4081000e-03 9.7963000e-04 /
CHEB / 3.5203000e-01 -2.7933000e-04 -1.9443000e-04 /
CHEB / 9.3310000e-02 -3.7396000e-04 -2.6009000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(1735)  -31.8 64.6  15.3  17.87 20.17 22.29 25.5  28.18 31.81
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!Here are the path reactions and their high-P limit kinetics:

sSPC(3071)+CH3(+m)=CH3O+sSPC(2810)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
43.5450802314256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3318000e+01 2.5661000e-07 1.7861000e-07 /
CHEB / -1.5036000e-01 4.8997000e-07 3.4104000e-07 /
CHEB / 3.7380000e-03 4.2687000e-07 2.9712000e-07 /
CHEB / 4.3257000e-02 3.4021000e-07 2.3681000e-07 /
CHEB / 1.9593000e-02 2.4843000e-07 1.7293000e-07 /

sSPC(1697)+HCO(+m)=CH3O+sSPC(2810)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
48.82466576771262 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2896000e+01 3.0417000e-07 2.1172000e-07 /
CHEB / -1.9465000e-01 5.7650000e-07 4.0127000e-07 /
CHEB / -2.6426000e-02 4.9246000e-07 3.4278000e-07 /
CHEB / 1.3985000e-02 3.8139000e-07 2.6547000e-07 /
CHEB / 1.5701000e-03 2.6902000e-07 1.8725000e-07 /

sSPC(1697)+HCO(+m)=sSPC(3071)+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
5.279585536287023 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7007000e+00 -6.9565000e-05 -4.8420000e-05 /
CHEB / 2.1728000e+00 1.6761000e-05 1.1667000e-05 /
CHEB / 8.0462000e-01 3.5776000e-05 2.4901000e-05 /
CHEB / 2.1913000e-01 9.3512000e-06 6.5087000e-06 /
CHEB / 5.6186000e-02 -5.7718000e-07 -4.0147000e-07 /

CH3O+sSPC(2810)(+m)=sSPC(1735)+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
24.088093654153845 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2084000e+00 1.1464000e-07 7.6732000e-08 /
CHEB / 1.1585000e+01 2.4000000e-07 1.6387000e-07 /
CHEB / 5.6320000e-01 2.4909000e-07 1.7531000e-07 /
CHEB / 2.1512000e-01 2.2704000e-07 1.6211000e-07 /
CHEB / 8.6438000e-02 1.7469000e-07 1.2414000e-07 /

sSPC(3071)+CH3(+m)=sSPC(1735)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
67.63317388557944 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0992000e+00 -8.1816000e-05 -5.6950000e-05 /
CHEB / 3.0210000e+00 7.7088000e-06 5.3663000e-06 /
CHEB / 1.0178000e+00 5.0579000e-05 3.5206000e-05 /
CHEB / 3.7317000e-01 1.8394000e-05 1.2803000e-05 /
CHEB / 1.2962000e-01 -1.6470000e-06 -1.1465000e-06 /
```

```
sSPC(1697)+HCO(+m)=sSPC(1735)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1058 (C2H4O3(1220))     deltaHrxn(T=298K) = -
72.91275942186647 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9730000e+00 -4.9264000e-05 -3.4292000e-05 /
CHEB / 2.7934000e+00 -3.3639000e-06 -2.3415000e-06 /
CHEB / 9.2965000e-01 2.9091000e-05 2.0250000e-05 /
CHEB / 3.3884000e-01 1.4710000e-05 1.0239000e-05 /
CHEB / 1.1385000e-01 1.5479000e-06 1.0774000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     nSPC(879)   -65.5 93.74 24.85 31.37 35.11 37.97 41.92 44.55 47.83
      null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(879)+HCO(+m)=nSPC(801)+sSPC(3071)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1135 (C3H4O6(1407))
      deltaHrxn(T=298K) = -5.9895386067030465 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6107000e+00 -7.5166000e-03 -5.1948000e-03 /
CHEB / 2.7702000e+00 8.5484000e-03 5.9023000e-03 /
CHEB / 7.6761000e-01 3.1306000e-04 2.2203000e-04 /
CHEB / 1.3399000e-01 -1.3731000e-03 -9.4608000e-04 /
CHEB / 1.6838000e-03 -2.1759000e-04 -1.5306000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH4               -17.9 44.47 8.43  9.84  11.14 12.41 15.0  17.25
      20.63 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!Here are the path reactions and their high-P limit kinetics:

CH3O+HCO(+m)=CH3+sSPC(2810)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
18.05833139205679 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2667000e+01 -1.2588000e-01 -7.8407000e-02 /
CHEB / -2.8735000e-01 1.3019000e-01 7.9650000e-02 /
CHEB / 8.2802000e-02 1.9223000e-02 1.3270000e-02 /
CHEB / 6.7814000e-02 -1.7721000e-02 -1.0211000e-02 /
CHEB / 2.6680000e-02 -8.6973000e-03 -5.8204000e-03 /

CH3+sSPC(2810)(+m)=CH3OH+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
70.92269381496183 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0414000e+01 -4.1714000e-01 -1.9450000e-01 /
CHEB / 1.2143000e+00 4.1931000e-01 1.7716000e-01 /
CHEB / 3.7098000e-01 6.1949000e-02 4.7025000e-02 /
CHEB / 1.4201000e-01 -3.6074000e-02 -1.0487000e-02 /
CHEB / 5.3986000e-02 -2.9163000e-02 -1.6519000e-02 /

CH3O+HCO(+m)=CH3OH+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
88.98102520701863 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1006000e+01 -1.3218000e-01 -8.2257000e-02 /
CHEB / 6.7038000e-01 1.3042000e-01 7.9596000e-02 /
CHEB / 2.1720000e-01 2.5680000e-02 1.7216000e-02 /
CHEB / 1.1726000e-01 -1.5615000e-02 -8.7180000e-03 /
CHEB / 5.5606000e-02 -1.0160000e-02 -6.6137000e-03 /

CH3+sSPC(2810)(+m)=CH4+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
108.44881470711489 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.2522000e+01 -4.2985000e-01 -2.0001000e-01 /
CHEB / 8.9608000e-02 4.1606000e-01 1.7422000e-01 /
CHEB / -1.7273000e-02 7.4602000e-02 5.2267000e-02 /
CHEB / 1.0325000e-02 -2.8300000e-02 -5.7467000e-03 /
CHEB / 8.4563000e-03 -2.9837000e-02 -1.5804000e-02 /

CH3O+HCO(+m)=CH4+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
126.50714609917168 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2690000e+01 -1.3495000e-01 -8.3964000e-02 /
CHEB / -2.3108000e-01 1.3004000e-01 7.9265000e-02 /
CHEB / -9.4905000e-02 2.8402000e-02 1.8876000e-02 /
CHEB / -2.9629000e-03 -1.4271000e-02 -7.8017000e-03 /
CHEB / 9.0966000e-03 -1.0500000e-02 -6.7620000e-03 /

CH3OH+CO(+m)=CH4+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1246 (C2H4O2(1259))    deltaHrxn(T=298K) = -
37.52612089215306 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3021000e+01 -8.9918000e-01 -2.1492000e-01 /
CHEB / 2.0380000e+01 7.8987000e-01 1.1658000e-01 /
CHEB / 5.5273000e-01 2.1582000e-01 1.0142000e-01 /
CHEB / 1.4624000e-01 -2.3667000e-02 3.0512000e-02 /
CHEB / 3.1139000e-02 -6.0001000e-02 -1.2371000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:
!     CO2+H=sSPC(2810)        5.2263889e+12      0.04600
5.0666667e+03
!     HCO+O=sSPC(2810)        1.0000000e+13      0.00000
0.0000000e+00

CO2+H(+m)=sSPC(2810)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1332 (CHO2J(1201)) High-P Limit: R_Addition_MultipleBond
```

```
estimate: (Average:) CO2     H_rad        deltaHrxn(T=298K) =
6.749892060549293 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3497000e+00 3.9543000e-01 -1.9138000e-01 /
CHEB / 4.2838000e+00 -2.7498000e-01 1.3368000e-01 /
CHEB / -2.4895000e-01 2.4406000e-02 1.7750000e-02 /
CHEB / -1.1215000e-01 1.2293000e-02 5.5416000e-03 /
CHEB / -6.4254000e-02 -7.8269000e-04 9.0909000e-03 /

HCO+O(+m)=sSPC(2810)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1332 (CHO2J(1201)) High-P Limit: Oa_R_Recombination
estimate: (Average:) CO_pri_rad     Oa          deltaHrxn(T=298K) = -
108.23853133691121 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2505000e+00 1.8393000e+01 -3.2941000e-01 /
CHEB / -3.0382000e+00 -3.3022000e+00 1.8001000e+00 /
CHEB / -9.6569000e-01 -1.6588000e+00 6.3847000e-01 /
CHEB / -2.2229000e-01 -7.6999000e-01 1.6159000e-01 /
CHEB / -1.4136000e-01 -2.0023000e-01 1.0407000e-01 /

HCO+O(+m)=CO2+H(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1332 (CHO2J(1201))     deltaHrxn(T=298K) = -114.98842339746051 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0373000e+01 1.4988000e-01 7.3249000e-02 /
CHEB / -2.7708000e+00 -1.4629000e-01 -5.7926000e-02 /
CHEB / -7.0961000e-01 -1.7635000e-02 -2.4823000e-02 /
CHEB / -2.3869000e-01 1.0948000e-02 5.7373000e-03 /
CHEB / -9.0578000e-02 7.5216000e-03 6.7332000e-03 /

CO+OH(+m)=sSPC(2810)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1332 (CHO2J(1201))     deltaHrxn(T=298K) = -
21.197160513559233 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6898000e-01 2.7477000e+00 -1.6399000e+00 /
CHEB / 5.6666000e+00 -1.5562000e+00 9.2336000e-01 /
CHEB / -4.6141000e-01 1.5209000e-01 4.4715000e-01 /
CHEB / -3.5408000e-01 1.9089000e-01 4.6375000e-03 /
CHEB / -1.7594000e-01 4.3613000e-02 -3.5533000e-02 /

!CO2+H(+m)=CO+OH(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1332 (CHO2J(1201))     deltaHrxn(T=298K) = 27.947052574108525 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 2.1225000e+00 -1.2374000e+00 -3.0478000e-01 /
!CHEB / 9.7444000e+00 1.1813000e-01 8.5036000e-02 /
!CHEB / -3.8839000e-02 3.0285000e-01 3.0743000e-03 /
!CHEB / -2.1750000e-02 1.4640000e-01 1.0782000e-02 /
!CHEB / -3.7033000e-02 4.1189000e-02 2.6673000e-02 /

HCO+O(+m)=CO+OH(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1332 (CHO2J(1201))     deltaHrxn(T=298K) = -87.04137082335197 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 1.1962000e+01 1.0021000e-01 3.5713000e-02 /
CHEB / -1.3269000e+00 -9.0061000e-02 -1.6940000e-02 /
CHEB / -3.5325000e-01 -1.6425000e-02 -2.1302000e-02 /
CHEB / -1.0404000e-01 4.4639000e-03 3.4130000e-05 /
CHEB / -2.5863000e-02 4.6533000e-03 4.0389000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3121)+O(+m)=sSPC(3071)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1472 (CH2O4JJ)   deltaHrxn(T=298K) = -3.9996309356562225
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0159000e+00 -2.6593000e-11 -1.8512000e-11 /
CHEB / 4.5803000e+00 -5.0973000e-11 -3.5479000e-11 /
CHEB / -4.3606000e-01 -4.4813000e-11 -3.1195000e-11 /
CHEB / -1.1378000e-01 -3.6029000e-11 -2.5078000e-11 /
CHEB / -8.0258000e-03 -2.6331000e-11 -1.8329000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+sSPC(2810)(+m)=CH2CO+sSPC(3071)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #11 (C3H3O4J(364))
      deltaHrxn(T=298K) = 3.94939017484419 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6475000e+00 -2.5588000e-01 -1.3219000e-01 /
CHEB / 2.5382000e+00 2.7263000e-01 1.3880000e-01 /
CHEB / 3.1693000e-02 3.1237000e-02 1.4080000e-02 /
CHEB / -6.0487000e-02 -3.9300000e-02 -1.2761000e-02 /
CHEB / -4.1112000e-02 -8.5304000e-03 -5.2352000e-03 /

CH2CO+sSPC(3071)(+m)=nSPC(801)+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #11 (C3H3O4J(364)) deltaHrxn(T=298K) = -
25.387718465918134 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9956000e+00 -1.2425000e-03 -8.7270000e-04 /
CHEB / 1.1658000e+01 4.5282000e-04 3.1461000e-04 /
CHEB / 6.1191000e-01 9.1142000e-04 6.4342000e-04 /
CHEB / 1.6419000e-01 1.5295000e-04 1.1013000e-04 /
CHEB / 3.0848000e-02 -1.4982000e-04 -1.0614000e-04 /

sSPC(1909)+sSPC(2810)(+m)=nSPC(801)+CO(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #11 (C3H3O4J(364))
      deltaHrxn(T=298K) = -21.438328291073944 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.2573000e+00 7.2341000e-05 4.5862000e-05 /
CHEB / 1.2283000e+01 5.1780000e-05 3.3489000e-05 /
CHEB / 4.4025000e-01 -2.3744000e-05 -1.0548000e-05 /
CHEB / 1.2508000e-01 -4.5540000e-05 -2.6453000e-05 /
CHEB / 3.2205000e-02 -4.3934000e-05 -3.0985000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!Here are the path reactions and their high-P limit kinetics:
```

```
HCO+sSPC(3071)(+m)=sSPC(2810)+sSPC(2810)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #31 (C2H2O4(415)) deltaHrxn(T=298K)
= -61.60341162348239 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2686000e+01 -5.3807000e-04 -3.7422000e-04 /
CHEB / -1.5157000e-02 -7.1213000e-04 -4.9510000e-04 /
CHEB / -2.2146000e-02 -4.3301000e-04 -3.0089000e-04 /
CHEB / 1.7477000e-02 -3.2971000e-04 -2.2906000e-04 /
CHEB / 4.1783000e-03 -2.6870000e-04 -1.8668000e-04 /

HCO+sSPC(3071)(+m)=CO+sSPC(3121)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #31 (C2H2O4(415))  deltaHrxn(T=298K) = -
83.04173988769575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0872000e+00 -4.4998000e-04 -3.1301000e-04 /
CHEB / 2.9549000e+00 -5.5826000e-04 -3.8822000e-04 /
CHEB / 8.9341000e-01 -3.2086000e-04 -2.2303000e-04 /
CHEB / 3.3809000e-01 -2.5000000e-04 -1.7375000e-04 /
CHEB / 1.2490000e-01 -2.0989000e-04 -1.4588000e-04 /

sSPC(2810)+sSPC(2810)(+m)=CO+sSPC(3121)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #31 (C2H2O4(415)) deltaHrxn(T=298K)
= -21.438328264213368 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4822000e+00 -2.2593000e-03 -1.5688000e-03 /
CHEB / 1.2836000e+01 -1.6723000e-03 -1.1583000e-03 /
CHEB / 6.1592000e-01 -3.3547000e-04 -2.3003000e-04 /
CHEB / 2.3768000e-01 -4.6457000e-04 -3.2053000e-04 /
CHEB / 9.8817000e-02 -6.0267000e-04 -4.1682000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:
```

```
nSPC(801)+H(+m)=CH3+OCOOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #44 (C2H4O3(522)) deltaHrxn(T=298K) = -3.219719183197462
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0358000e+01 -8.0808000e-05 -5.6246000e-05 /
CHEB / 1.7024000e+00 5.9774000e-05 4.1604000e-05 /
CHEB / 7.1307000e-01 2.7673000e-05 1.9261000e-05 /
CHEB / 2.1957000e-01 -5.0531000e-06 -3.5167000e-06 /
CHEB / 8.0060000e-02 -7.1613000e-06 -4.9844000e-06 /

CH3+OCOOH(+m)=CH3CO+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #44 (C2H4O3(522)) deltaHrxn(T=298K) = -11.9281982109016
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0673000e+01 -1.2393000e-04 -8.6260000e-05 /
CHEB / 4.6078000e-01 8.8674000e-05 6.1718000e-05 /
CHEB / 3.7057000e-01 4.8607000e-05 3.3830000e-05 /
CHEB / 1.6521000e-01 -8.0648000e-06 -5.6123000e-06 /
CHEB / 6.1225000e-02 -1.3088000e-05 -9.1086000e-06 /

nSPC(801)+H(+m)=CH3CO+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #44 (C2H4O3(522)) deltaHrxn(T=298K) = -15.147917394099062
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1544000e+01 -9.3345000e-05 -6.4971000e-05 /
CHEB / 4.1517000e-01 6.2125000e-05 4.3241000e-05 /
CHEB / 4.1146000e-01 3.8927000e-05 2.7094000e-05 /
CHEB / 1.7854000e-01 -4.1098000e-06 -2.8601000e-06 /
CHEB / 6.5526000e-02 -1.0221000e-05 -7.1135000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3121)+O(+m)=sSPC(2810)+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #64 (CH2O4JJ(576))      deltaHrxn(T=298K) = -
25.79706394778344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.0716000e+01 -7.5541000e-07 -5.2582000e-07 /
CHEB / 1.4124000e+00 -1.4683000e-06 -1.0221000e-06 /
CHEB / 4.2081000e-02 -1.3473000e-06 -9.3782000e-07 /
CHEB / 2.4929000e-02 -1.1647000e-06 -8.1074000e-07 /
CHEB / 1.3467000e-02 -9.4319000e-07 -6.5653000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C2H3O-2           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1909)+H(+m)=CH3+CO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
105.84916902096776 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3727000e+01 2.9870000e-06 2.0929000e-06 /
CHEB / 5.2767000e-02 -2.8557000e-06 -2.0034000e-06 /
CHEB / 9.3612000e-03 -8.6573000e-07 -6.0763000e-07 /
CHEB / 5.4680000e-02 1.7027000e-06 1.1925000e-06 /
CHEB / 3.1960000e-02 1.2730000e-06 8.8880000e-07 /

CH2CO+OH(+m)=CH3+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
57.21408390768698 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2412000e+00 -4.5795000e-01 -1.9457000e-01 /
CHEB / 2.3962000e+00 5.3659000e-01 2.0393000e-01 /
CHEB / 2.3689000e-01 -7.8822000e-03 3.0013000e-02 /
CHEB / 9.6510000e-03 -6.7916000e-02 -2.9686000e-02 /
CHEB / -5.4026000e-03 -1.5906000e-02 -1.5540000e-02 /
```

```
C2H3O-2+O(+m)=CH3+CO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
148.26500421002174 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2031000e+01 7.2715000e-05 5.0621000e-05 /
CHEB / 5.9924000e-01 -5.3562000e-05 -3.7290000e-05 /
CHEB / -7.5668000e-02 -1.9912000e-05 -1.3860000e-05 /
CHEB / -6.0824000e-02 4.7966000e-06 3.3405000e-06 /
CHEB / -4.3451000e-02 5.0011000e-06 3.4812000e-06 /

sSPC(1909)+H(+m)=C2H3O-2+O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) =
42.415835189053965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.0821000e+00 -7.9659000e-05 -5.5464000e-05 /
CHEB / 1.4162000e+01 2.6805000e-05 1.8670000e-05 /
CHEB / 4.3054000e-01 5.0700000e-05 3.5300000e-05 /
CHEB / 3.1493000e-01 7.3687000e-06 5.1260000e-06 /
CHEB / 1.6662000e-01 -8.0975000e-06 -5.6399000e-06 /

C2H3O-2+O(+m)=CH2CO+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
91.05092030233476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2762000e+01 6.8525000e-05 4.7704000e-05 /
CHEB / -2.4851000e-01 -5.5660000e-05 -3.8750000e-05 /
CHEB / -1.2950000e-01 -2.0714000e-05 -1.4418000e-05 /
CHEB / -4.7097000e-03 4.2178000e-06 2.9376000e-06 /
CHEB / 1.4828000e-02 4.8643000e-06 3.3858000e-06 /

CH3CO+O(+m)=CH2CO+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
59.284231640104586 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7174000e+00 -3.0910000e-05 -2.1584000e-05 /
CHEB / 2.2196000e+00 1.0496000e-07 9.5189000e-08 /
CHEB / 3.1457000e-01 2.5987000e-05 1.8156000e-05 /
CHEB / 1.1884000e-01 9.7306000e-06 6.7794000e-06 /
CHEB / 3.7668000e-02 -4.5727000e-06 -3.2079000e-06 /

C2H3O-2+O(+m)=CH3CO+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (C2H3O2J(468))      deltaHrxn(T=298K) = -
31.766688662230173 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3217000e+00 -1.5286000e-04 -1.0641000e-04 /
CHEB / 3.2400000e+00 8.4622000e-05 5.8911000e-05 /
CHEB / 4.4537000e-01 8.2148000e-05 5.7182000e-05 /
CHEB / 1.3923000e-01 -3.1042000e-07 -2.1895000e-07 /
CHEB / 2.5783000e-02 -1.6894000e-05 -1.1760000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!Here are the path reactions and their high-P limit kinetics:

OCOOH+CO(+m)=CO2+sSPC(2810)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #204 (C2HO4J(619))      deltaHrxn(T=298K) = -
81.19112154669637 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1874000e+01 -2.7465000e-07 -1.9117000e-07 /
CHEB / 1.9399000e+01 -5.3872000e-07 -3.7499000e-07 /
CHEB / 4.5655000e-01 -5.0741000e-07 -3.5320000e-07 /
CHEB / 1.9294000e-01 -4.5659000e-07 -3.1782000e-07 /
CHEB / 8.1084000e-02 -3.8823000e-07 -2.7024000e-07 /

CO+sSPC(3071)(+m)=CO2+sSPC(2810)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #204 (C2HO4J(619)) deltaHrxn(T=298K) = -
80.5315278622335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7189000e+00 -2.7466000e-07 -1.9119000e-07 /
CHEB / 6.6863000e-01 -5.3875000e-07 -3.7501000e-07 /
CHEB / -6.3119000e-03 -5.0744000e-07 -3.5322000e-07 /
CHEB / 1.4218000e-03 -4.5662000e-07 -3.1784000e-07 /
CHEB / -4.5413000e-03 -3.8825000e-07 -2.7025000e-07 /

CO+sSPC(3071)(+m)=OCOOH+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #204 (C2HO4J(619))      deltaHrxn(T=298K) =
0.6595936844628554 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1430000e+01 -2.7464000e-07 -1.9117000e-07 /
CHEB / 4.1230000e+01 -5.3872000e-07 -3.7499000e-07 /
CHEB / 5.8767000e-01 -5.0741000e-07 -3.5319000e-07 /
CHEB / 2.1571000e-01 -4.5659000e-07 -3.1782000e-07 /
CHEB / 8.1111000e-02 -3.8822000e-07 -2.7023000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     acetone     -51.56      70.09 17.97 22.0  25.89 29.34 34.93 39.15
      44.77 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1590)+HCO(+m)=sSPC(2810)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #252 (C4H6O3(684))
      deltaHrxn(T=298K) = -18.908325070330417 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0680000e+01 -9.7592000e-01 -1.6670000e-01 /
CHEB / 4.7609000e-01 9.4645000e-01 8.0634000e-02 /
CHEB / 6.2727000e-02 1.9444000e-01 1.0926000e-01 /
CHEB / -1.0900000e-01 -7.6071000e-02 2.3936000e-02 /
CHEB / -5.9903000e-02 -7.9062000e-02 -2.5069000e-02 /

sSPC(2810)+CH2C[O]CH3(+m)=CO2+acetone(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #252 (C4H6O3(684)) deltaHrxn(T=298K) = -
104.3893348172605 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1053000e+01 -1.3448000e+00 -8.0782000e-02 /
CHEB / 8.7377000e-01 9.9622000e-01 -5.2438000e-02 /
CHEB / -4.9485000e-02 4.6300000e-01 6.4523000e-02 /
CHEB / -2.5429000e-01 7.4970000e-02 8.2186000e-02 /
CHEB / -1.8326000e-01 -7.6537000e-02 3.4228000e-02 /

sSPC(1590)+HCO(+m)=CO2+acetone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #252 (C4H6O3(684))      deltaHrxn(T=298K) = -
123.29765988759092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1817000e+01 -1.0035000e+00 -1.8894000e-01 /
CHEB / -9.4656000e-02 9.1080000e-01 8.1541000e-02 /
CHEB / -2.0113000e-01 2.4940000e-01 1.1735000e-01 /
CHEB / -1.8286000e-01 -3.8317000e-02 4.3594000e-02 /
CHEB / -9.6430000e-02 -7.8647000e-02 -1.5951000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!Here are the path reactions and their high-P limit kinetics:

CO+sSPC(1356)(+m)=CO2+sSPC(1590)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #320 (C4H5O4J(677))      deltaHrxn(T=298K) = -
67.9627961820027 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5142000e+00 -6.6297000e-08 -4.6148000e-08 /
CHEB / 1.3582000e-02 -1.3004000e-07 -9.0517000e-08 /
CHEB / -6.3113000e-03 -1.2247000e-07 -8.5251000e-08 /
CHEB / 1.4223000e-03 -1.1020000e-07 -7.6705000e-08 /
CHEB / -4.5408000e-03 -9.3688000e-08 -6.5214000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H5OJ(8)         -7.6  73.85 18.59 21.98 24.96 27.55 32.16 35.44
      39.21 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!Here are the path reactions and their high-P limit kinetics:
```

```
CH2CO+CH3CO(+m)=C3H5OJ(8)+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #387 (C4H5O2J(872))     deltaHrxn(T=298K) = -
20.398213169537513 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2442000e+01 -2.0346000e-04 -1.4161000e-04 /
CHEB / 2.9668000e+01 1.2394000e-05 8.6297000e-06 /
CHEB / 3.5416000e-01 2.8966000e-05 2.0162000e-05 /
CHEB / 9.0825000e-02 -2.4175000e-05 -1.6822000e-05 /
CHEB / -1.2359000e-03 -3.3773000e-05 -2.3502000e-05 /

CO+CH2C[O]CH3(+m)=C3H5OJ(8)+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #387 (C4H5O2J(872))     deltaHrxn(T=298K) = -
4.6896727954532444 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8176000e+01 -2.0976000e-04 -1.4599000e-04 /
CHEB / 3.4754000e+01 2.3573000e-06 1.6452000e-06 /
CHEB / 2.4779000e-01 2.2341000e-05 1.5552000e-05 /
CHEB / 5.2173000e-02 -2.8954000e-05 -2.0148000e-05 /
CHEB / -1.3746000e-02 -3.7421000e-05 -2.6040000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+CH2CO(+m)=CO+CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #522 (C4H5O2J(818))     deltaHrxn(T=298K) = -
15.708540374084269 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4917000e+01 -1.3507000e-04 -9.4008000e-05 /
CHEB / 3.1458000e+01 -5.3088000e-05 -3.6942000e-05 /
CHEB / 2.7706000e-01 -3.8651000e-05 -2.6895000e-05 /
CHEB / 7.9849000e-02 -3.2700000e-05 -2.2754000e-05 /
CHEB / 1.5965000e-02 -9.1592000e-06 -6.3715000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+H(+m)=iC4H8+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #632 (C4H9O2J(1004))    deltaHrxn(T=298K) = -
30.306259462150294 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3118000e+01 -1.6156000e-01 -9.8126000e-02 /
CHEB / -2.8878000e-03 1.4928000e-01 8.7364000e-02 /
CHEB / -2.9276000e-01 2.0693000e-02 1.4286000e-02 /
CHEB / -1.8592000e-01 -1.9079000e-02 -1.0082000e-02 /
CHEB / -1.2250000e-01 -6.0714000e-03 -4.0679000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
```

```
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+iC4H7=tSPC(54)       2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+sC3H5=tSPC(54)      1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(54)=tSPC(77)       1.1250000e+11      0.00000
2.4400000e+04
!     CH2OOH+aC3H4=tSPC(77)   1.9263655e+11      0.04067
9.2900000e+03
!     C4H7OJ(79)+O=tSPC(54)   1.0000000e+13      0.00000
0.0000000e+00

tSPC(77)(+m)=tSPC(54)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = 1.7383281845795295E-4
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6915000e+00 9.3117000e-01 -1.0185000e-01 /
CHEB / 5.7532000e-01 9.4322000e-01 1.1994000e-02 /
CHEB / -4.5087000e+00 -4.1343000e-02 6.0607000e-02 /
CHEB / -2.3252000e+00 -4.3289000e-01 1.2717000e-03 /
CHEB / -8.4203000e-01 -3.4589000e-01 -3.9447000e-02 /

O2+iC4H7(+m)=tSPC(54)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/Cd       deltaHrxn(T=298K) = -
21.837999719838262 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6130000e+00 9.7016000e-01 -8.3096000e-02 /
CHEB / -4.6543000e+00 1.0739000e+00 3.9504000e-02 /
CHEB / -2.9062000e+00 1.9217000e-01 6.9161000e-02 /
CHEB / -1.4648000e+00 -1.5602000e-01 1.3728000e-03 /
CHEB / -5.5781000e-01 -1.4475000e-01 -2.9858000e-02 /

O2+iC4H7(+m)=tSPC(77)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -21.83817355265672
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0303000e+00 -9.5785000e-02 -2.1218000e-01 /
CHEB / -2.4684000e+00 1.8192000e+00 3.8624000e-02 /
CHEB / -2.8746000e+00 4.3958000e-01 7.0636000e-02 /
CHEB / -1.7879000e+00 -9.8064000e-02 4.1450000e-02 /
CHEB / -7.9253000e-01 -1.9517000e-01 2.0685000e-02 /

nSPC(102)+sC3H5(+m)=tSPC(54)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     Cd_rad/NonDe          deltaHrxn(T=298K) = -
99.0199183766068 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1025000e+01 1.2350000e+01 -4.8300000e-01 /
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CHEB / -3.7040000e+00 2.9692000e-01 2.7072000e-01 /
CHEB / -3.3532000e+00 -1.7108000e-01 4.4774000e-01 /
CHEB / -2.0711000e+00 -2.6115000e-01 3.1791000e-01 /
CHEB / -1.0494000e+00 -1.2595000e-01 1.3196000e-01 /

nSPC(102)+sC3H5(+m)=tSPC(77)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -99.02009220942526
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3643000e+00 1.2512000e+01 -4.5868000e-01 /
CHEB / -4.9100000e+00 1.9120000e-01 2.5140000e-01 /
CHEB / -3.7889000e+00 -2.2596000e-01 4.2970000e-01 /
CHEB / -2.1851000e+00 -2.5051000e-01 3.0884000e-01 /
CHEB / -1.0877000e+00 -8.2312000e-02 1.2935000e-01 /

nSPC(102)+sC3H5(+m)=O2+iC4H7(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -77.18191865676853
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2997000e+01 5.4213000e-06 3.7740000e-06 /
CHEB / -4.7484000e-01 8.2463000e-06 5.7412000e-06 /
CHEB / -1.2892000e-01 1.0431000e-06 7.2587000e-07 /
CHEB / -7.5448000e-02 -3.1277000e-06 -2.1781000e-06 /
CHEB / -5.3953000e-02 -3.7570000e-06 -2.6158000e-06 /

CH2OOH+aC3H4(+m)=tSPC(54)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -48.07495516518735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1071000e-01 3.6524000e+00 -9.4225000e-01 /
CHEB / -3.2047000e+00 3.0943000e+00 5.8974000e-02 /
CHEB / -4.2649000e+00 1.1039000e+00 2.3975000e-01 /
CHEB / -2.3092000e+00 -2.7756000e-02 2.4732000e-01 /
CHEB / -9.7569000e-01 -2.7476000e-01 1.3482000e-01 /

CH2OOH+aC3H4(+m)=tSPC(77)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_rad/H2/O     Ca_Cd/H2          deltaHrxn(T=298K)
= -48.0751289980058 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2545000e+00 3.8091000e+00 -9.1192000e-01 /
CHEB / -4.4055000e+00 2.9774000e+00 4.5656000e-02 /
CHEB / -4.6938000e+00 1.0369000e+00 2.3053000e-01 /
CHEB / -2.4175000e+00 -2.6430000e-02 2.4516000e-01 /
CHEB / -1.0091000e+00 -2.3974000e-01 1.3839000e-01 /

CH2OOH+aC3H4(+m)=O2+iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -26.236955445349082
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7442000e+00 -4.5625000e-01 -2.4550000e-01 /
CHEB / 2.5362000e+00 5.8069000e-01 2.6285000e-01 /
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CHEB / -4.2079000e-01 4.9828000e-03 5.3202000e-02 /
CHEB / -2.3095000e-01 -1.2372000e-01 -3.9894000e-02 /
CHEB / -9.7100000e-02 -5.1130000e-02 -4.0081000e-02 /

nSPC(102)+sC3H5(+m)=CH2OOH+aC3H4(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (tSPC(54))      deltaHrxn(T=298K) = -
50.94496321141945 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1135000e+00 -2.2969000e-03 -1.6065000e-03 /
CHEB / 6.5559000e-01 1.9968000e-03 1.3976000e-03 /
CHEB / 2.5867000e-01 6.9552000e-04 4.8635000e-04 /
CHEB / 6.3942000e-02 -1.8658000e-04 -1.3165000e-04 /
CHEB / -6.3446000e-03 -1.9201000e-04 -1.3448000e-04 /

C4H7OJ(79)+O(+m)=tSPC(54)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/NonDe     Oa       deltaHrxn(T=298K) = -
59.29384248830546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0391000e+00 4.7618000e+00 -1.5159000e-01 /
CHEB / -6.0477000e+00 1.6644000e+00 -6.2905000e-01 /
CHEB / -3.7834000e+00 7.8893000e-01 6.2719000e-02 /
CHEB / -1.9740000e+00 9.0692000e-02 3.1559000e-01 /
CHEB / -7.9358000e-01 -1.6946000e-01 2.4489000e-01 /

C4H7OJ(79)+O(+m)=tSPC(77)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -59.29401632112392
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9677000e+00 3.6781000e+00 -9.4844000e-01 /
CHEB / -6.5870000e+00 2.7517000e+00 6.6282000e-03 /
CHEB / -4.1252000e+00 9.7292000e-01 2.1747000e-01 /
CHEB / -2.1922000e+00 -1.5303000e-02 2.3386000e-01 /
CHEB / -9.1462000e-01 -2.3458000e-01 1.2994000e-01 /

C4H7OJ(79)+O(+m)=O2+iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -37.45584276846719
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3609000e+01 -5.1026000e-04 -4.3228000e-04 /
CHEB / -6.2147000e-01 6.2568000e-04 5.2137000e-04 /
CHEB / -7.4536000e-02 5.3250000e-05 4.5412000e-05 /
CHEB / -5.2065000e-02 -1.6636000e-04 -1.3490000e-04 /
CHEB / -3.8352000e-02 -3.1120000e-05 -2.2272000e-05 /

nSPC(102)+sC3H5(+m)=C4H7OJ(79)+O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (tSPC(54))      deltaHrxn(T=298K) = -
39.72607588830133 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0017000e+01 -1.1872000e-03 -8.2635000e-04 /
CHEB / 8.6128000e-01 9.1306000e-04 6.3552000e-04 /
CHEB / 4.1183000e-01 4.1304000e-04 2.8749000e-04 /
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CHEB / 1.2890000e-01 -1.6724000e-05 -1.1637000e-05 /
CHEB / 1.5703000e-02 -8.5094000e-05 -5.9226000e-05 /

C4H7OJ(79)+O(+m)=CH2OOH+aC3H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -11.218887323118118
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5615000e+00 -3.9411000e-01 -1.6924000e-01 /
CHEB / 2.4161000e+00 4.8260000e-01 1.9097000e-01 /
CHEB / 4.4273000e-01 -3.3620000e-02 1.0106000e-02 /
CHEB / 4.0220000e-02 -5.6998000e-02 -2.7880000e-02 /
CHEB / -1.0630000e-02 -1.0648000e-02 -1.0263000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+O(+m)=sSPC(1590)+CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #951 (C4H7O2J(698))     deltaHrxn(T=298K) = -
13.608201147764106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0262000e+00 -3.6931000e-05 -2.5707000e-05 /
CHEB / 2.9868000e+00 2.1476000e-05 1.4949000e-05 /
CHEB / 9.8206000e-01 1.6557000e-05 1.1524000e-05 /
CHEB / 2.3688000e-01 9.2088000e-07 6.4104000e-07 /
CHEB / 2.6812000e-02 -2.0865000e-06 -1.4523000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H7       32.3 69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!Here are the path reactions and their high-P limit kinetics:

tSPC(77)+tSPC(54)(+m)=iC4H7+tSPC(122)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1155 (C8H14O4(388))     deltaHrxn(T=298K) = -
3.8864543583372324E-8 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2720000e+00 -5.5068000e-01 -1.7487000e-01 /
CHEB / 3.3613000e+00 6.8202000e-01 1.8632000e-01 /
CHEB / 3.7044000e-01 -4.1364000e-02 3.5086000e-02 /
CHEB / -5.7177000e-02 -1.0191000e-01 -3.9318000e-02 /
CHEB / -4.6138000e-02 -1.5715000e-02 -2.0929000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C8H15J(44)  19.61 110.6 42.15 51.82 60.89 68.87 81.78 91.51 106.68
      null
!     C8H14       3.28  104.5 41.02 51.34 60.44 68.08 80.22 89.2  102.98
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:
!     C8H14+H=C8H15J(44)      4.9400000e+13      0.00000
1.5000000e+03
!     iC4H8+iC4H7=C8H15J(44)  5.0381048e+11      0.00000
1.5645000e+04
```

```
C8H14+H(+m)=C8H15J(44)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1271 (C8H15J(44)) High-P Limit: R_Addition_MultipleBond
exact:  Cd/H2_Cd/Nd2     H_rad      deltaHrxn(T=298K) = -
32.66619391109151 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9474000e+00 2.7479000e+00 -7.4310000e-01 /
CHEB / -6.7060000e+00 1.3935000e+00 2.9127000e-01 /
CHEB / -4.6610000e+00 7.6036000e-02 2.3139000e-01 /
CHEB / -2.4914000e+00 -3.4963000e-01 3.8155000e-02 /
CHEB / -1.1163000e+00 -2.2042000e-01 -6.3596000e-02 /

iC4H8+iC4H7(+m)=C8H15J(44)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1271 (C8H15J(44)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/Nd2     C_rad/H2/Cd
      deltaHrxn(T=298K) = -8.889114004657301 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1136000e+00 1.3033000e+00 -2.8300000e-01 /
CHEB / -1.6167000e+00 1.2107000e+00 2.5900000e-02 /
CHEB / -4.3248000e+00 1.4667000e-01 1.4674000e-01 /
CHEB / -2.4435000e+00 -2.7152000e-01 4.7343000e-02 /
CHEB / -1.1364000e+00 -2.0597000e-01 -4.0758000e-02 /

C8H14+H(+m)=iC4H8+iC4H7(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1271 (C8H15J(44))      deltaHrxn(T=298K) = -
23.77707990643421 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2475000e+01 -6.6524000e-01 -1.9773000e-01 /
CHEB / 1.2424000e+00 7.6616000e-01 1.8780000e-01 /
CHEB / -6.6729000e-02 4.1395000e-02 7.0021000e-02 /
CHEB / -9.1496000e-02 -1.2741000e-01 -3.5338000e-02 /
CHEB / -2.3420000e-02 -5.9851000e-02 -4.1475000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sC3H5            61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3              35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     HO2              3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
```

```
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!Here are the path reactions and their high-P limit kinetics:
!     sC3H5+CH2OOH=C4H8O2(62) 1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7+HO2=C4H8O2(62)    1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(77)+H=C4H8O2(62)   5.0000000e+13      0.00000
0.0000000e+00
!     C4H7OJ(79)+OH=C4H8O2(62)      2.0000000e+13      0.00000
0.0000000e+00
!     tSPC(54)+H=C4H8O2(62)   1.4157154e+13      -0.15000
2.9166667e+02

sC3H5+CH2OOH(+m)=C4H8O2(62)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62)) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_rad/H2/O          deltaHrxn(T=298K) = -
99.01991835655028 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0821000e+00 7.6175000e+00 9.4153000e-01 /
CHEB / -3.6283000e+00 6.6628000e-01 3.4646000e-02 /
CHEB / -2.3331000e+00 5.8727000e-02 -1.2481000e-02 /
CHEB / -1.1655000e+00 -5.4404000e-02 -1.4387000e-02 /
CHEB / -5.6627000e-01 -6.9434000e-02 -1.5876000e-02 /

iC4H7+HO2(+m)=C4H8O2(62)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     O_rad/NonDe          deltaHrxn(T=298K) = -
60.32424250236001 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4798000e+00 3.6860000e+00 -5.3609000e-01 /
CHEB / -4.0512000e+00 5.4026000e-01 2.5451000e-01 /
CHEB / -2.3374000e+00 2.1782000e-01 1.0226000e-01 /
CHEB / -1.2052000e+00 -5.0833000e-02 -1.1735000e-03 /
CHEB / -5.9982000e-01 -9.4927000e-02 -1.6197000e-02 /

sC3H5+CH2OOH(+m)=iC4H7+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -38.69567585419026
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0941000e+01 -6.0934000e-04 -4.2464000e-04 /
CHEB / -1.2222000e-01 5.4787000e-04 3.8185000e-04 /
CHEB / 1.6856000e-01 1.8201000e-04 1.2685000e-04 /
CHEB / 7.8407000e-02 -7.4125000e-05 -5.1732000e-05 /
CHEB / 2.9077000e-02 -4.8213000e-05 -3.3605000e-05 /

tSPC(77)+H(+m)=C4H8O2(62)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
88.190497830169 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0651000e+00 7.1573000e+00 6.6172000e-01 /
CHEB / -3.6704000e+00 4.4165000e-01 -7.2035000e-02 /
CHEB / -2.3426000e+00 1.9535000e-02 -1.6864000e-02 /
CHEB / -1.1570000e+00 -6.4236000e-02 -1.1905000e-02 /
CHEB / -5.5686000e-01 -7.6829000e-02 -1.7168000e-02 /

tSPC(77)+H(+m)=sC3H5+CH2OOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = 10.829420526381284
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8568000e+00 -1.5479000e-03 -1.0766000e-03 /
CHEB / 6.1688000e+00 1.6905000e-03 1.1756000e-03 /
CHEB / 8.4081000e-01 1.1853000e-04 8.2534000e-05 /
CHEB / 2.6702000e-01 -2.3559000e-04 -1.6374000e-04 /
CHEB / 9.4898000e-02 -5.2019000e-05 -3.6245000e-05 /

tSPC(77)+H(+m)=iC4H7+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -27.86625532780898
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1571000e+01 -2.7848000e-03 -1.9468000e-03 /
CHEB / 1.9451000e-01 2.8757000e-03 2.0113000e-03 /
CHEB / 2.5649000e-01 4.9756000e-04 3.4735000e-04 /
CHEB / 1.0703000e-01 -5.0817000e-04 -3.5634000e-04 /
CHEB / 4.4641000e-02 -1.4702000e-04 -1.0243000e-04 /

C4H7OJ(79)+OH(+m)=C4H8O2(62)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
44.44533746473968 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2379000e+01 7.2383000e-01 -5.3673000e-02 /
CHEB / -3.6107000e+00 1.0276000e+00 -1.0795000e-02 /
CHEB / -2.0346000e+00 3.9099000e-01 5.4378000e-02 /
CHEB / -1.1691000e+00 1.8114000e-02 3.6525000e-02 /
CHEB / -6.1295000e-01 -8.0729000e-02 -9.4683000e-04 /

sC3H5+CH2OOH(+m)=C4H7OJ(79)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -54.574580891810584
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3155000e+01 2.6617000e-06 1.8538000e-06 /
CHEB / -4.0744000e-01 -2.1433000e-06 -1.4930000e-06 /
CHEB / -1.6025000e-02 -7.6122000e-07 -5.3000000e-07 /
CHEB / 9.5289000e-03 7.8911000e-08 5.5096000e-08 /
CHEB / 5.1316000e-03 1.4670000e-07 1.0212000e-07 /

iC4H7+HO2(+m)=C4H7OJ(79)+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -15.878905037620324
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.3085000e+01 -1.8183000e-01 -1.1012000e-01 /
CHEB / -3.1539000e-01 2.1965000e-01 1.3024000e-01 /
CHEB / -2.2817000e-02 -6.1620000e-03 -6.2348000e-04 /
CHEB / -2.0046000e-02 -3.6125000e-02 -2.0219000e-02 /
CHEB / 2.6365000e-04 -1.9950000e-03 -3.1054000e-03 /

tSPC(77)+H(+m)=C4H7OJ(79)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -43.7451603654293
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4087000e+01 -5.3710000e-06 -5.2932000e-06 /
CHEB / -2.8266000e-01 4.4807000e-06 4.4202000e-06 /
CHEB / 1.5245000e-02 5.2229000e-06 4.6429000e-06 /
CHEB / 3.0562000e-02 -4.1546000e-06 -3.5648000e-06 /
CHEB / 2.0994000e-02 -1.9520000e-06 -1.7042000e-06 /

tSPC(54)+H(+m)=C4H8O2(62)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
88.19067166298746 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2493000e-01 7.1573000e+00 6.6172000e-01 /
CHEB / -4.0329000e+00 4.4165000e-01 -7.2035000e-02 /
CHEB / -2.3747000e+00 1.9535000e-02 -1.6864000e-02 /
CHEB / -1.1760000e+00 -6.4236000e-02 -1.1905000e-02 /
CHEB / -5.7267000e-01 -7.6829000e-02 -1.7168000e-02 /

tSPC(54)+H(+m)=sC3H5+CH2OOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = 10.829246693562823
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2166000e+00 -1.5479000e-03 -1.0766000e-03 /
CHEB / 5.8062000e+00 1.6905000e-03 1.1756000e-03 /
CHEB / 8.0867000e-01 1.1853000e-04 8.2534000e-05 /
CHEB / 2.4803000e-01 -2.3559000e-04 -1.6374000e-04 /
CHEB / 7.9087000e-02 -5.2019000e-05 -3.6245000e-05 /

tSPC(54)+H(+m)=iC4H7+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -27.86642916062744
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0931000e+01 -2.7848000e-03 -1.9468000e-03 /
CHEB / -1.6805000e-01 2.8757000e-03 2.0113000e-03 /
CHEB / 2.2436000e-01 4.9756000e-04 3.4735000e-04 /
CHEB / 8.8046000e-02 -5.0817000e-04 -3.5634000e-04 /
CHEB / 2.8830000e-02 -1.4702000e-04 -1.0243000e-04 /

tSPC(54)+H(+m)=tSPC(77)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -1.7383281845440024E-4
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 4.4230000e+00 -4.1074000e-03 -2.8473000e-03 /
CHEB / 4.0842000e+00 4.9769000e-03 3.4474000e-03 /
CHEB / 1.1070000e+00 -3.9269000e-04 -2.6822000e-04 /
CHEB / 3.3208000e-01 -4.5999000e-04 -3.1987000e-04 /
CHEB / 1.1085000e-01 -1.2628000e-04 -8.8009000e-05 /

tSPC(54)+H(+m)=C4H7OJ(79)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O2(62))   deltaHrxn(T=298K) = -43.74533419824776
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3446000e+01 -5.3710000e-06 -5.2932000e-06 /
CHEB / -6.4522000e-01 4.4807000e-06 4.4202000e-06 /
CHEB / -1.6889000e-02 5.2229000e-06 4.6429000e-06 /
CHEB / 1.1576000e-02 -4.1546000e-06 -3.5648000e-06 /
CHEB / 5.1823000e-03 -1.9520000e-06 -1.7042000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C8H14       3.28  104.5 41.02 51.34 60.44 68.08 80.22 89.2  102.98
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     C5H9J(9)    40.44 84.58 25.93 32.15 37.71 42.43 49.97 55.63 64.41
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C8H13J(41)  36.74 103.31      40.11 50.37 59.12 66.37 77.84 86.33
      99.18 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!Here are the path reactions and their high-P limit kinetics:
!     sC3H5+C5H9J(9)=C8H14    1.4157154e+13      -0.15000
2.9166667e+02
!     C8H13J(41)+H=C8H14      5.0000000e+13      0.00000
0.0000000e+00
!     iC4H7+iC4H7=C8H14 1.1500000e+13      0.00000     0.0000000e+00

sC3H5+C5H9J(9)(+m)=C8H14(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_rad/H2/Cs         deltaHrxn(T=298K) = -
98.70003535933742 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2365000e+01 7.5191000e-01 -1.2936000e-01 /
CHEB / -1.7094000e+00 9.5013000e-01 -2.7233000e-02 /
CHEB / -7.3831000e-01 3.6284000e-01 8.0283000e-02 /
CHEB / -2.9599000e-01 1.9779000e-02 6.8819000e-02 /
CHEB / -8.8047000e-02 -7.4158000e-02 1.9202000e-02 /
```

```
C8H13J(41)+H(+m)=C8H14(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
82.45110539492794 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3262000e+01 5.5018000e-01 -6.9597000e-02 /
CHEB / -1.1948000e+00 9.0006000e-01 -7.7807000e-02 /
CHEB / -7.1281000e-01 4.9029000e-01 1.9013000e-02 /
CHEB / -3.1754000e-01 1.3676000e-01 6.4604000e-02 /
CHEB / -1.0448000e-01 -3.5153000e-02 4.9349000e-02 /

C8H13J(41)+H(+m)=sC3H5+C5H9J(9)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14)     deltaHrxn(T=298K) = 16.248929964409477
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7855000e+00 -1.0570000e+00 -1.3992000e-01 /
CHEB / 7.3102000e+00 1.0205000e+00 3.6641000e-02 /
CHEB / 5.4397000e-01 2.2105000e-01 1.1133000e-01 /
CHEB / 3.5484000e-02 -1.0345000e-01 3.3962000e-02 /
CHEB / -3.1481000e-02 -1.0401000e-01 -2.6033000e-02 /

iC4H7+iC4H7(+m)=C8H14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_rad/H2/Cd          deltaHrxn(T=298K) = -
61.31372987451952 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2848000e+01 3.8188000e-01 -4.1132000e-02 /
CHEB / -9.9314000e-01 6.9166000e-01 -6.5993000e-02 /
CHEB / -6.4527000e-01 5.0774000e-01 -2.7460000e-02 /
CHEB / -4.2378000e-01 2.8835000e-01 1.0658000e-02 /
CHEB / -2.3648000e-01 1.0801000e-01 3.0264000e-02 /

sC3H5+C5H9J(9)(+m)=iC4H7+iC4H7(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14)     deltaHrxn(T=298K) = -37.38630548481791
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2083000e+01 -1.1425000e+00 -1.2929000e-01 /
CHEB / 6.8164000e-01 1.0158000e+00 7.5430000e-03 /
CHEB / 1.2412000e-01 2.9527000e-01 1.0168000e-01 /
CHEB / -1.0549000e-01 -6.1784000e-02 5.3079000e-02 /
CHEB / -8.4575000e-02 -1.0965000e-01 -8.2971000e-03 /

C8H13J(41)+H(+m)=iC4H7+iC4H7(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1462 (C8H14)     deltaHrxn(T=298K) = -21.137375520408426
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2020000e+01 -1.3178000e+00 -7.3104000e-02 /
CHEB / 1.8281000e+00 1.0390000e+00 -5.5329000e-02 /
CHEB / 2.5584000e-01 4.3182000e-01 5.9909000e-02 /
CHEB / -1.1356000e-01 1.5078000e-03 7.6629000e-02 /
CHEB / -8.8774000e-02 -1.2224000e-01 2.5494000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(157)   -4.85 104.09      37.36 44.83 50.46 55.08 61.65 66.34
      72.86 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(122)+H(+m)=HO2+tSPC(77)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1551 (C4H8O4(372))     deltaHrxn(T=298K) = -
30.306433296019485 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1253000e+01 -9.6323000e-03 -6.6471000e-03 /
CHEB / -1.1276000e-01 1.0714000e-02 7.3858000e-03 /
CHEB / 1.7492000e-01 6.3573000e-04 4.4430000e-04 /
CHEB / 1.0253000e-01 -1.9646000e-03 -1.3504000e-03 /
CHEB / 4.2662000e-02 -3.8720000e-04 -2.7097000e-04 /

tSPC(157)+H(+m)=HO2+tSPC(77)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1551 (C4H8O4(372))     deltaHrxn(T=298K) = -
29.676310570215897 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1645000e+01 -9.6323000e-03 -6.6471000e-03 /
CHEB / 4.6879000e-01 1.0714000e-02 7.3858000e-03 /
CHEB / 2.1267000e-01 6.3573000e-04 4.4430000e-04 /
CHEB / 1.3289000e-01 -1.9646000e-03 -1.3504000e-03 /
CHEB / 6.6297000e-02 -3.8720000e-04 -2.7097000e-04 /

tSPC(122)+H(+m)=tSPC(157)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1551 (C4H8O4(372))     deltaHrxn(T=298K) = -
0.630122725803588 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4184000e+00 -4.8654000e-03 -3.3700000e-03 /
CHEB / 2.6650000e+00 5.9136000e-03 4.0929000e-03 /
CHEB / 6.7977000e-01 -4.9822000e-04 -3.4087000e-04 /
CHEB / 1.9171000e-01 -7.5960000e-04 -5.2661000e-04 /
CHEB / 5.3665000e-02 -7.0265000e-05 -4.9912000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!Here are the path reactions and their high-P limit kinetics:

iC4H7+tSPC(54)(+m)=C4H7OJ(79)+C4H7OJ(79)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1642 (C8H14O2(387))
      deltaHrxn(T=298K) = -18.938011478214904 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2821000e+01 -6.4480000e-01 -1.8578000e-01 /
CHEB / 2.8194000e-02 7.4430000e-01 1.7463000e-01 /
CHEB / -4.2907000e-02 2.1293000e-02 6.1140000e-02 /
CHEB / -7.4140000e-02 -1.0643000e-01 -2.9229000e-02 /
CHEB / -2.7459000e-02 -4.5391000e-02 -2.9236000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3              35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tC4H9       14.3  76.21 21.71 26.64 31.62 36.12 43.55 49.22 58.13
!     O2               0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     OC[CH3]3    -23.14      76.55 26.22 32.91 38.66 43.41 50.9  56.36
      64.83 null
!     iC4H8       -2.22 70.16 21.12 26.15 30.77 34.8  41.35 46.34 54.27
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tBuOH       -75.1 78.01 27.2  34.21 40.27 45.3  53.28 59.16 68.42
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     O(48)            59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
```

```
iC4H8+tSPC(97)(+m)=tBuOH+tSPC(54)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C8H17O3J(364)) deltaHrxn(T=298K) = -
0.24000937996347815 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2707000e+01 -6.5459000e-01 -1.7764000e-01 /
CHEB / 1.9300000e+01 8.1336000e-01 1.7420000e-01 /
CHEB / 9.9231000e-01 -5.1391000e-02 6.2008000e-02 /
CHEB / 1.2069000e-01 -1.2328000e-01 -4.6672000e-02 /
CHEB / 9.1166000e-03 -1.8314000e-02 -3.0111000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(439)+iC4H8(+m)=C4H8O2(62)+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1741 (C8H17O3J(574))
      deltaHrxn(T=298K) = 1.3399028688399177 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.4710000e+00 -3.2853000e-02 -2.4445000e-02 /
CHEB / 1.6444000e+01 4.4281000e-02 3.2919000e-02 /
CHEB / 2.7272000e-01 -7.7216000e-03 -5.6676000e-03 /
CHEB / 5.9118000e-02 -6.2091000e-03 -4.6908000e-03 /
CHEB / -1.0253000e-03 1.1976000e-03 8.9630000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

HOC[CH2][CH3]2+tSPC(122)(+m)=tSPC(97)+tSPC(77)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1967 (C8H16O5(518))
      deltaHrxn(T=298K) = -14.238590453591769 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8393000e+00 -5.7597000e-01 -1.8127000e-01 /
CHEB / 1.7603000e+00 7.0446000e-01 1.9015000e-01 /
CHEB / 3.4846000e-01 -2.5853000e-02 4.1213000e-02 /
CHEB / -6.8290000e-02 -1.1370000e-01 -4.0639000e-02 /
CHEB / -5.6234000e-02 -2.1319000e-02 -2.4798000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3C[OH]CH3 -22.33      74.56 21.77 26.05 29.95 33.3  38.64 42.68
      49.13
```

```
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H2CCCH3[OH] -39.44      69.6  20.59 25.3  29.06 32.04 36.55 39.89
      45.32
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+HOC[CH2][CH3]2=tSPC(97)    2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+CH3C[OH]CH3=tSPC(97)      3.5900000e+14      -0.75000
0.0000000e+00
!     tSPC(54)+H2O=tSPC(97)   1.2500000e+03      2.76000
4.8500000e+04
!     tSPC(97)=tSPC(439)      5.0760000e+08      1.32000
2.1500000e+04
!     CH2OOH+H2CCCH3[OH]=tSPC(439)  2.4827386e+10      0.24400
1.0487500e+04
!     C4H8O2(62)+OH=tSPC(439) 2.7100000e+12      0.00000
0.0000000e+00

tSPC(439)(+m)=tSPC(97)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -12.898513750882664
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4153000e+00 1.7617000e+00 -1.6333000e-01 /
CHEB / -4.6662000e+00 3.0350000e-01 1.0669000e-01 /
CHEB / -5.5715000e+00 -9.8073000e-02 -2.7386000e-02 /
CHEB / -2.3641000e+00 -2.6728000e-01 -7.0263000e-02 /
CHEB / -6.3053000e-01 -1.7377000e-01 -3.9474000e-02 /

O2+HOC[CH2][CH3]2(+m)=tSPC(97)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/Cs       deltaHrxn(T=298K) = -
34.53611050144967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5321000e+00 7.7928000e-01 -3.2723000e-02 /
CHEB / -8.2127000e+00 1.1554000e+00 -1.4678000e-02 /
CHEB / -4.8941000e+00 3.6250000e-01 3.5539000e-02 /
CHEB / -2.4400000e+00 -1.9291000e-01 1.5611000e-02 /
CHEB / -7.8664000e-01 -2.7994000e-01 -2.1233000e-02 /

O2+HOC[CH2][CH3]2(+m)=tSPC(439)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -21.63759675056701
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 9.1393000e+00 7.4276000e-01 -7.2063000e-02 /
CHEB / -4.1069000e+00 1.1588000e+00 2.2347000e-02 /
CHEB / -2.9468000e+00 3.2764000e-01 7.8905000e-03 /
CHEB / -1.9687000e+00 -1.3941000e-01 3.3150000e-02 /
CHEB / -1.0096000e+00 -2.5163000e-01 -1.4150000e-03 /

nSPC(102)+CH3C[OH]CH3(+m)=tSPC(97)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     C_rad/NDMustO         deltaHrxn(T=298K) = -
87.37094132014758 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4837000e+00 1.0140000e+01 -5.9262000e-01 /
CHEB / -1.0097000e+01 -2.2871000e-01 5.9909000e-01 /
CHEB / -5.5636000e+00 -6.7110000e-01 2.6573000e-01 /
CHEB / -2.5802000e+00 -6.1487000e-01 3.9249000e-02 /
CHEB / -8.3115000e-01 -2.9980000e-01 -5.5102000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=tSPC(439)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
74.47242756926491 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7780000e+00 1.0274000e+01 -5.1547000e-01 /
CHEB / -6.1300000e+00 -4.6408000e-01 4.7685000e-01 /
CHEB / -3.5834000e+00 -6.5185000e-01 2.6772000e-01 /
CHEB / -2.0918000e+00 -5.3004000e-01 8.1652000e-02 /
CHEB / -1.0615000e+00 -2.8409000e-01 -4.2309000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=O2+HOC[CH2][CH3]2(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -52.834830818697895 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3100000e+01 -1.1025000e-02 -9.5439000e-03 /
CHEB / -1.2641000e+00 1.5585000e-02 1.3296000e-02 /
CHEB / -2.5054000e-01 -3.3455000e-03 -2.6396000e-03 /
CHEB / -1.2037000e-01 -2.2852000e-03 -1.9671000e-03 /
CHEB / -7.2499000e-02 4.3681000e-04 3.1201000e-04 /

tSPC(54)+H2O(+m)=tSPC(97)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97)) High-P Limit: 1,3_Insertion_ROR exact:
Cd/H2_Cd/Nd2     H_OH         deltaHrxn(T=298K) = -14.178203645345512
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5767000e+01 4.6583000e+00 -8.7658000e-01 /
CHEB / 7.8901000e+00 1.2440000e+00 4.4468000e-01 /
CHEB / -5.1567000e+00 3.6677000e-02 1.7889000e-01 /
CHEB / -2.4650000e+00 -3.9074000e-01 -1.8703000e-03 /
CHEB / -7.5588000e-01 -3.1253000e-01 -6.0446000e-02 /

tSPC(439)(+m)=tSPC(54)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = 1.279689894462848
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -1.4261000e+01 4.7907000e+00 -8.0240000e-01 /
CHEB / 1.1616000e+01 1.0115000e+00 3.2666000e-01 /
CHEB / -3.4295000e+00 5.4385000e-02 1.7958000e-01 /
CHEB / -2.0629000e+00 -3.0589000e-01 4.0284000e-02 /
CHEB / -1.0023000e+00 -2.9631000e-01 -4.7379000e-02 /

O2+HOC[CH2][CH3]2(+m)=tSPC(54)+H2O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
20.357906856104165 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4839000e+00 -2.7098000e-01 -1.5264000e-01 /
CHEB / 9.6495000e+00 3.2615000e-01 1.7591000e-01 /
CHEB / 8.8480000e-02 -1.2394000e-03 1.1418000e-02 /
CHEB / -1.7559000e-02 -5.4108000e-02 -3.1137000e-02 /
CHEB / -1.8134000e-02 -1.8973000e-02 -1.5506000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=tSPC(54)+H2O(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -73.19273767480206 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8406000e+00 -4.7530000e-02 -3.2397000e-02 /
CHEB / 1.2918000e+00 5.8258000e-02 3.9537000e-02 /
CHEB / 6.2505000e-01 -3.5647000e-03 -2.1503000e-03 /
CHEB / 1.5376000e-01 -8.0173000e-03 -5.5268000e-03 /
CHEB / -1.9579000e-03 -9.2435000e-04 -7.0046000e-04 /

CH2OOH+H2CCCH3[OH](+m)=tSPC(97)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -34.16623517440169
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7886000e+00 1.6714000e+00 -2.9898000e-01 /
CHEB / -4.4420000e+00 1.6656000e+00 6.1283000e-02 /
CHEB / -5.1566000e+00 3.0965000e-01 1.0146000e-01 /
CHEB / -2.4714000e+00 -3.0469000e-01 2.0720000e-02 /
CHEB / -7.6310000e-01 -3.0736000e-01 -3.9213000e-02 /

CH2OOH+H2CCCH3[OH](+m)=tSPC(439)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) C_rad/H2/O     Cd/Nd2_Cd/H2      deltaHrxn(T=298K)
= -21.267721423519028 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6824000e+00 2.1370000e+00 -3.6922000e-03 /
CHEB / -7.3756000e-01 9.7338000e-01 -3.4810000e-01 /
CHEB / -3.1173000e+00 4.2074000e-01 1.3562000e-01 /
CHEB / -1.9505000e+00 -1.5604000e-01 1.2071000e-01 /
CHEB / -1.0044000e+00 -3.0827000e-01 -3.1636000e-02 /

O2+HOC[CH2][CH3]2(+m)=CH2OOH+H2CCCH3[OH](+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -0.36987532704797843 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 7.3375000e+00 -8.3704000e-01 -2.0623000e-01 /
CHEB / 4.0778000e+00 9.8190000e-01 1.9440000e-01 /
CHEB / -2.1331000e-01 2.4184000e-02 7.6998000e-02 /
CHEB / -2.5347000e-01 -1.5246000e-01 -3.8374000e-02 /
CHEB / -1.3841000e-01 -7.0850000e-02 -4.5272000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=CH2OOH+H2CCCH3[OH](+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -53.20470614574588 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0678000e+01 -2.8163000e-02 -2.1512000e-02 /
CHEB / -4.1602000e-01 3.5114000e-02 2.6890000e-02 /
CHEB / -1.1350000e-01 -2.5424000e-03 -2.0233000e-03 /
CHEB / -8.7038000e-02 -5.1050000e-03 -3.9384000e-03 /
CHEB / -7.3066000e-02 -5.9876000e-04 -4.0659000e-04 /

CH2OOH+H2CCCH3[OH](+m)=tSPC(54)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
19.988031529056187 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7383000e+00 -3.2942000e-01 -1.7479000e-01 /
CHEB / 1.0994000e+01 3.9693000e-01 2.0168000e-01 /
CHEB / 2.4610000e-01 -1.1969000e-02 6.8228000e-03 /
CHEB / -2.6157000e-02 -5.7891000e-02 -3.1359000e-02 /
CHEB / -5.2193000e-02 -1.2130000e-02 -1.0675000e-02 /

C4H8O2(62)+OH(+m)=tSPC(97)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -45.22494029137742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7649000e+00 1.6714000e+00 -2.9898000e-01 /
CHEB / -8.3733000e+00 1.6656000e+00 6.1283000e-02 /
CHEB / -5.1913000e+00 3.0965000e-01 1.0146000e-01 /
CHEB / -2.4861000e+00 -3.0469000e-01 2.0720000e-02 /
CHEB / -7.7257000e-01 -3.0736000e-01 -3.9213000e-02 /

C4H8O2(62)+OH(+m)=tSPC(439)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/Nd2_Cd/H2     O_pri_rad       deltaHrxn(T=298K)
= -32.326426540494765 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6587000e+00 2.1370000e+00 -3.6922000e-03 /
CHEB / -4.6688000e+00 9.7338000e-01 -3.4810000e-01 /
CHEB / -3.1520000e+00 4.2074000e-01 1.3562000e-01 /
CHEB / -1.9652000e+00 -1.5604000e-01 1.2071000e-01 /
CHEB / -1.0139000e+00 -3.0827000e-01 -3.1636000e-02 /

C4H8O2(62)+OH(+m)=O2+HOC[CH2][CH3]2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
10.688829789927752 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1948000e+01 -8.3704000e-01 -2.0623000e-01 /
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CHEB / 1.5609000e-01 9.8190000e-01 1.9440000e-01 /
CHEB / -3.2189000e-01 2.4184000e-02 7.6998000e-02 /
CHEB / -3.0171000e-01 -1.5246000e-01 -3.8374000e-02 /
CHEB / -1.5955000e-01 -7.0850000e-02 -4.5272000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=C4H8O2(62)+OH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -42.146001028770144 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1713000e+01 -2.8163000e-02 -2.1512000e-02 /
CHEB / -6.0588000e-01 3.5114000e-02 2.6890000e-02 /
CHEB / -1.6340000e-01 -2.5424000e-03 -2.0233000e-03 /
CHEB / -1.0452000e-01 -5.1050000e-03 -3.9384000e-03 /
CHEB / -7.9947000e-02 -5.9876000e-04 -4.0659000e-04 /

C4H8O2(62)+OH(+m)=tSPC(54)+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -31.046736646031917
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2380000e+00 -3.2942000e-01 -1.7479000e-01 /
CHEB / 7.0625000e+00 3.9693000e-01 2.0168000e-01 /
CHEB / 2.1141000e-01 -1.1969000e-02 6.8228000e-03 /
CHEB / -4.0794000e-02 -5.7891000e-02 -3.1359000e-02 /
CHEB / -6.1665000e-02 -1.2130000e-02 -1.0675000e-02 /

C4H8O2(62)+OH(+m)=CH2OOH+H2CCCH3[OH](+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
11.058705116975734 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8003000e+00 -2.5635000e-01 -4.7387000e-02 /
CHEB / 2.1755000e+00 2.6497000e-01 2.4043000e-02 /
CHEB / 1.0246000e-01 5.3493000e-02 4.0698000e-02 /
CHEB / -1.2703000e-01 -4.3901000e-02 5.4103000e-05 /
CHEB / -1.1417000e-01 -3.1732000e-02 -1.8350000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     tSPC(157)   -4.85 104.09      37.36 44.83 50.46 55.08 61.65 66.34
      72.86 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
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!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+tSPC(77)=tSPC(122)   2.2600000e+12      0.00000
0.0000000e+00
!     tSPC(122)=tSPC(157)     3.4152599e+09      1.20000
3.8255000e+04
!     tSPC(122)=tSPC(157)     4.6000000e+04      2.11000
1.5470000e+04
!     tSPC(213)+OH=tSPC(157)  2.3501400e+11      0.30815
4.9629937e+03

tSPC(157)(+m)=tSPC(122)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122))    deltaHrxn(T=298K) = 0.6301227258035924
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5441000e+01 2.1369000e+00 -4.5127000e-02 /
CHEB / 9.2113000e+00 1.2322000e-01 -3.1253000e-02 /
CHEB / -3.1065000e+00 1.5571000e-03 -1.2533000e-02 /
CHEB / -1.3940000e+00 -3.1032000e-02 -1.0737000e-02 /
CHEB / -6.0125000e-01 -6.7491000e-03 -9.6098000e-03 /

O2+tSPC(77)(+m)=tSPC(122)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/Cd       deltaHrxn(T=298K) = -
18.938067655329846 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0041000e+01 1.1008000e+00 -9.4177000e-02 /
CHEB / -5.8039000e+00 1.1456000e+00 3.6529000e-02 /
CHEB / -3.0926000e+00 1.6545000e-01 5.5386000e-02 /
CHEB / -1.5745000e+00 -9.4286000e-02 -2.3801000e-02 /
CHEB / -7.0019000e-01 -4.8292000e-02 -3.1241000e-02 /

O2+tSPC(77)(+m)=tSPC(157)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122))    deltaHrxn(T=298K) = -19.568190381133437
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8581000e+00 1.1043000e+00 -9.4817000e-02 /
CHEB / 5.2344000e+00 1.0925000e+00 6.1260000e-02 /
CHEB / -2.4858000e+00 1.3289000e-01 6.9764000e-02 /
CHEB / -1.3437000e+00 -1.0919000e-01 -1.7349000e-02 /
CHEB / -6.1011000e-01 -6.0222000e-02 -2.5903000e-02 /

tSPC(122)(+m)=tSPC(213)+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122))    deltaHrxn(T=298K) = -32.687084774094416
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.1643000e+00 7.7417000e-01 -3.8426000e-02 /
CHEB / 1.0463000e+00 9.4837000e-01 2.5343000e-02 /
CHEB / -2.8102000e+00 2.0745000e-01 3.5089000e-02 /
CHEB / -1.4565000e+00 -8.0773000e-02 -1.3898000e-02 /
CHEB / -6.7589000e-01 -5.5488000e-02 -2.8255000e-02 /

tSPC(157)(+m)=tSPC(213)+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122))    deltaHrxn(T=298K) = -32.05696204829083
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5214000e+00 2.0000000e+00 -1.2181000e-08 /
CHEB / -1.3297000e+00 -3.4670000e-08 -2.3752000e-08 /
CHEB / -3.4556000e+00 -3.2114000e-08 -2.1995000e-08 /
CHEB / -1.4828000e+00 -2.8170000e-08 -1.9287000e-08 /
CHEB / -6.4270000e-01 -2.3226000e-08 -1.5894000e-08 /

O2+tSPC(77)(+m)=tSPC(213)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(122))    deltaHrxn(T=298K) = -51.62515242942426
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0838000e+01 -7.0355000e-01 -1.2385000e-01 /
CHEB / 6.7683000e-01 8.9117000e-01 1.1717000e-01 /
CHEB / 3.0896000e-02 -7.8446000e-02 5.2087000e-02 /
CHEB / 1.7894000e-02 -1.3288000e-01 -3.6208000e-02 /
CHEB / 3.4298000e-02 -1.3253000e-02 -2.3249000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
```

```
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

tSPC(439)+O2(+m)=tSPC(122)+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O5J(339)) deltaHrxn(T=298K) = -17.65855159368546
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4104000e-01 -2.6531000e-01 -1.4734000e-01 /
CHEB / 1.0896000e+01 3.3202000e-01 1.7640000e-01 /
CHEB / 1.6427000e-01 -2.3769000e-02 -3.7009000e-04 /
CHEB / 1.3954000e-02 -5.1237000e-02 -3.0131000e-02 /
CHEB / 2.5629000e-04 -5.2051000e-03 -7.6556000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(157)   -4.85 104.09      37.36 44.83 50.46 55.08 61.65 66.34
      72.86 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(157)+O(+m)=tSPC(213)+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3959 (C4H7O5J(702))    deltaHrxn(T=298K) = -
99.85961212944744 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3949000e+01 -4.0837000e-06 -2.8425000e-06 /
CHEB / -1.1808000e+00 -7.3046000e-06 -5.0845000e-06 /
CHEB / -2.1924000e-01 -5.1225000e-06 -3.5657000e-06 /
CHEB / -1.3547000e-01 -2.5402000e-06 -1.7682000e-06 /
CHEB / -7.8779000e-02 -4.2729000e-07 -2.9742000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     tSPC(343)   -9.84 83.82 25.39 30.56 34.79 38.21 43.57 47.08 51.06
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     iC4H5OJ(15) 8.76  72.88 22.52 27.78 31.88 35.05 39.89 43.1  46.9
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     tSPC(343)+OH=tSPC(213)  2.0000000e+13      0.00000
0.0000000e+00
!     HO2+iC4H5OJ(15)=tSPC(213)     1.4157154e+13      -0.15000
2.9166667e+02
!     CH2OOH+tSPC(346)=tSPC(213)    1.4157154e+13      -0.15000
2.9166667e+02

tSPC(343)+OH(+m)=tSPC(213)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4220 (tSPC(213)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
45.07524014699175 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1891000e+01 7.0085000e-01 -4.5825000e-02 /
CHEB / -3.5486000e+00 1.0396000e+00 -1.4801000e-02 /
CHEB / -2.2612000e+00 4.2592000e-01 5.0349000e-02 /
CHEB / -1.3159000e+00 2.6578000e-02 3.7050000e-02 /
CHEB / -6.7699000e-01 -9.7873000e-02 -1.7220000e-04 /

HO2+iC4H5OJ(15)(+m)=tSPC(213)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4220 (tSPC(213)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     C_rad/H2/Cd          deltaHrxn(T=298K) = -
54.78455039678781 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0361000e+01 1.6821000e+00 -3.3365000e-01 /
CHEB / -4.3374000e+00 1.1286000e+00 1.7489000e-01 /
CHEB / -2.5265000e+00 3.7796000e-01 7.5241000e-02 /
CHEB / -1.3654000e+00 -3.4208000e-02 2.0932000e-02 /
CHEB / -6.7629000e-01 -1.0889000e-01 -9.2771000e-03 /

HO2+iC4H5OJ(15)(+m)=tSPC(343)+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4220 (tSPC(213))  deltaHrxn(T=298K) = -
9.709310249796053 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / 1.2780000e+01 -5.8800000e-01 -1.7180000e-01 /
CHEB / 5.6621000e-02 7.0536000e-01 1.7683000e-01 /
CHEB / -5.7591000e-02 -2.0195000e-02 3.4481000e-02 /
CHEB / -7.7056000e-02 -1.0098000e-01 -2.7786000e-02 /
CHEB / -9.3402000e-03 -1.7675000e-02 -1.8828000e-02 /

CH2OOH+tSPC(346)(+m)=tSPC(213)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4220 (tSPC(213)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     Cd_rad/OneDe          deltaHrxn(T=298K) = -
87.98095365132187 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4417000e-01 7.0747000e+00 4.7504000e-01 /
CHEB / -4.4954000e+00 3.0786000e-01 -6.4153000e-02 /
CHEB / -2.7294000e+00 -4.3033000e-03 3.1923000e-03 /
CHEB / -1.3702000e+00 -8.0565000e-02 -4.0662000e-03 /
CHEB / -6.5097000e-01 -9.0519000e-02 -1.4097000e-02 /

CH2OOH+tSPC(346)(+m)=tSPC(343)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4220 (tSPC(213))  deltaHrxn(T=298K) = -
42.90571350433011 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3186000e+01 -6.6864000e-05 -5.9207000e-05 /
CHEB / -4.6276000e-01 7.0952000e-05 6.2557000e-05 /
CHEB / -3.0667000e-02 2.4721000e-05 2.1599000e-05 /
CHEB / -8.1115000e-03 -3.3737000e-05 -2.8982000e-05 /
CHEB / -8.9659000e-03 -5.4947000e-06 -4.8583000e-06 /

CH2OOH+tSPC(346)(+m)=HO2+iC4H5OJ(15)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4220 (tSPC(213))  deltaHrxn(T=298K) = -
33.196403254534054 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1207000e+01 -2.5206000e-03 -1.7807000e-03 /
CHEB / -9.7538000e-02 2.7324000e-03 1.9325000e-03 /
CHEB / 1.3333000e-01 3.5255000e-04 2.4811000e-04 /
CHEB / 4.0693000e-02 -5.4483000e-04 -3.8812000e-04 /
CHEB / 3.3658000e-03 -1.2901000e-04 -8.9995000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(97)+H(+m)=HO2+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) = -
16.067842842427716 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0018000e+01 -6.2348000e-02 -4.0645000e-02 /
CHEB / 7.5663000e-01 7.5553000e-02 4.8855000e-02 /
CHEB / 4.9908000e-01 -3.4599000e-03 -1.7557000e-03 /
CHEB / 1.5556000e-01 -1.2506000e-02 -8.0964000e-03 /
CHEB / 3.3894000e-02 -6.3560000e-04 -6.4440000e-04 /

tSPC(439)+H(+m)=HO2+HOC[CH2][CH3]2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) = -
28.96635659331038 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1669000e+01 -1.8085000e-02 -1.2387000e-02 /
CHEB / 5.5210000e-01 2.0448000e-02 1.3976000e-02 /
CHEB / 4.4298000e-01 7.3564000e-04 5.2962000e-04 /
CHEB / 1.8114000e-01 -3.8722000e-03 -2.6372000e-03 /
CHEB / 5.5278000e-02 -5.8216000e-04 -4.1440000e-04 /

tSPC(439)+H(+m)=tSPC(97)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4396 (C4H10O3(454))    deltaHrxn(T=298K) = -
12.898513750882664 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2753000e-01 -1.4911000e-02 -1.0233000e-02 /
CHEB / 1.0478000e+00 1.7888000e-02 1.2251000e-02 /
CHEB / 6.0322000e-01 -8.7382000e-04 -5.7169000e-04 /
CHEB / 1.6445000e-01 -2.9883000e-03 -2.0473000e-03 /
CHEB / 2.2505000e-02 -7.4043000e-05 -6.3865000e-05 /

CH2OOH+CH3C[OH]CH3(+m)=HO2+HOC[CH2][CH3]2(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4396 (C4H10O3(454))
      deltaHrxn(T=298K) = -17.577890002323834 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4230000e+00 -6.2348000e-02 -4.0645000e-02 /
CHEB / 6.4796000e-01 7.5553000e-02 4.8855000e-02 /
CHEB / 3.8673000e-01 -3.4599000e-03 -1.7557000e-03 /
CHEB / 7.0077000e-02 -1.2506000e-02 -8.0964000e-03 /
CHEB / -2.0591000e-02 -6.3560000e-04 -6.4440000e-04 /
```

```
tSPC(97)+H(+m)=CH2OOH+CH3C[OH]CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) =
1.5100471598961143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7507000e+00 -3.7753000e-02 -2.5200000e-02 /
CHEB / 3.3491000e+00 4.7943000e-02 3.1817000e-02 /
CHEB / 9.0026000e-01 -5.9297000e-03 -3.6818000e-03 /
CHEB / 2.2113000e-01 -6.3595000e-03 -4.3006000e-03 /
CHEB / 4.1715000e-02 3.3559000e-04 1.4588000e-04 /

tSPC(439)+H(+m)=CH2OOH+CH3C[OH]CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) = -
11.38846659098655 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2543000e+00 -1.4911000e-02 -1.0233000e-02 /
CHEB / 2.2371000e+00 1.7888000e-02 1.2251000e-02 /
CHEB / 9.1578000e-01 -8.7382000e-04 -5.7169000e-04 /
CHEB / 2.7395000e-01 -2.9883000e-03 -2.0473000e-03 /
CHEB / 6.5606000e-02 -7.4043000e-05 -6.3865000e-05 /

HO2+HOC[CH2][CH3]2(+m)=C4H8O2(62)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) = -
54.18500856591421 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3370000e+00 -2.9378000e-01 -1.4177000e-01 /
CHEB / 2.7969000e+00 3.6220000e-01 1.6542000e-01 /
CHEB / 7.9071000e-01 -2.6183000e-02 1.1014000e-03 /
CHEB / 1.5266000e-01 -5.0336000e-02 -2.5849000e-02 /
CHEB / 2.3285000e-02 -5.2678000e-03 -6.6672000e-03 /

tSPC(97)+H(+m)=C4H8O2(62)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4396 (C4H10O3(454))    deltaHrxn(T=298K) = -
70.25285140834193 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3876000e+00 -6.6028000e-02 -4.2944000e-02 /
CHEB / 1.8860000e+00 7.8531000e-02 5.0653000e-02 /
CHEB / 7.7996000e-01 -1.4992000e-03 -4.8002000e-04 /
CHEB / 2.7378000e-01 -1.3503000e-02 -8.6728000e-03 /
CHEB / 8.8611000e-02 -1.2945000e-03 -1.0861000e-03 /

tSPC(439)+H(+m)=C4H8O2(62)+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4396 (C4H10O3(454))    deltaHrxn(T=298K) = -
83.15136515922458 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8845000e+00 -1.8668000e-02 -1.2783000e-02 /
CHEB / 1.8137000e+00 2.0789000e-02 1.4205000e-02 /
CHEB / 7.3963000e-01 1.1395000e-03 8.0485000e-04 /
CHEB / 2.9514000e-01 -3.9797000e-03 -2.7076000e-03 /
CHEB / 1.0751000e-01 -7.1776000e-04 -5.0694000e-04 /
```

```
CH2OOH+CH3C[OH]CH3(+m)=C4H8O2(62)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4396 (C4H10O3(454))     deltaHrxn(T=298K) = -
71.76289856823804 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7930000e+00 -6.6028000e-02 -4.2944000e-02 /
CHEB / 1.7773000e+00 7.8531000e-02 5.0653000e-02 /
CHEB / 6.6762000e-01 -1.4992000e-03 -4.8002000e-04 /
CHEB / 1.8830000e-01 -1.3503000e-02 -8.6728000e-03 /
CHEB / 3.4127000e-02 -1.2945000e-03 -1.0861000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C8H15J(44)  19.61 110.6 42.15 51.82 60.89 68.87 81.78 91.51 106.68
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     C5H9J(9)    40.44 84.58 25.93 32.15 37.71 42.43 49.97 55.63 64.41
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C8H14       3.28  104.5 41.02 51.34 60.44 68.08 80.22 89.2  102.98
      null
!Here are the path reactions and their high-P limit kinetics:

OH+C8H15J(44)(+m)=CH3C[OH]CH3+C5H9J(9)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4513 (C8H16O(519))
      deltaHrxn(T=298K) = -11.588520748725536 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5780000e+00 -1.3837000e+00 -3.8907000e-02 /
CHEB / 3.3223000e+00 1.0273000e+00 -3.9558000e-02 /
CHEB / 4.6001000e-01 5.5137000e-01 3.4143000e-02 /
CHEB / -4.0920000e-01 9.5789000e-02 6.9243000e-02 /
CHEB / -3.0030000e-01 -1.3831000e-01 3.9180000e-02 /
```

```
OH+C8H15J(44)(+m)=HOC[CH2][CH3]2+iC4H7(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4513 (C8H16O(519))
      deltaHrxn(T=298K) = -22.72731231139697 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9501000e+00 -1.4001000e+00 -3.4990000e-02 /
CHEB / 2.6036000e+00 1.0120000e+00 -3.6382000e-02 /
CHEB / 4.3237000e-01 5.6855000e-01 2.9896000e-02 /
CHEB / -3.8733000e-01 1.2600000e-01 6.4172000e-02 /
CHEB / -3.0987000e-01 -1.2424000e-01 3.8872000e-02 /

CH3C[OH]CH3+C5H9J(9)(+m)=HOC[CH2][CH3]2+iC4H7(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4513 (C8H16O(519))
      deltaHrxn(T=298K) = -11.138791562671443 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0845000e+00 -1.4218000e+00 -2.9540000e-02 /
CHEB / 3.8580000e+00 9.9031000e-01 -3.1777000e-02 /
CHEB / 4.3829000e-01 5.8849000e-01 2.3737000e-02 /
CHEB / -4.6106000e-01 1.6538000e-01 5.5420000e-02 /
CHEB / -3.5958000e-01 -1.0259000e-01 3.6579000e-02 /

OH+C8H15J(44)(+m)=C4H8O-i1+iC4H8(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4513 (C8H16O(519))      deltaHrxn(T=298K) = -
70.98238925389121 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9258000e+00 -1.4046000e+00 -3.3661000e-02 /
CHEB / 3.0674000e+00 1.0078000e+00 -3.5089000e-02 /
CHEB / 5.8268000e-01 5.7357000e-01 2.8836000e-02 /
CHEB / -3.2211000e-01 1.3489000e-01 6.2449000e-02 /
CHEB / -2.8880000e-01 -1.2001000e-01 3.8258000e-02 /

CH3C[OH]CH3+C5H9J(9)(+m)=C4H8O-i1+iC4H8(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4513 (C8H16O(519))
      deltaHrxn(T=298K) = -59.393868505165685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1432000e+00 -1.4263000e+00 -2.8047000e-02 /
CHEB / 4.2291000e+00 9.8586000e-01 -3.0206000e-02 /
CHEB / 6.0479000e-01 5.9316000e-01 2.2646000e-02 /
CHEB / -3.9277000e-01 1.7455000e-01 5.3150000e-02 /
CHEB / -3.4042000e-01 -9.7519000e-02 3.5315000e-02 /

HOC[CH2][CH3]2+iC4H7(+m)=C4H8O-i1+iC4H8(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4513 (C8H16O(519))
      deltaHrxn(T=298K) = -48.25507694249424 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0141000e+00 -1.4431000e+00 -2.3115000e-02 /
CHEB / 6.3168000e+00 9.6830000e-01 -2.5275000e-02 /
CHEB / 7.2778000e-01 6.0769000e-01 1.8160000e-02 /
CHEB / -4.1220000e-01 2.0655000e-01 4.4422000e-02 /
CHEB / -3.6858000e-01 -7.7510000e-02 3.0692000e-02 /
```

```
OH+C8H15J(44)(+m)=H2O+C8H14(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4513 (C8H16O(519))     deltaHrxn(T=298K) = -
83.44150043302727 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9611000e+00 -1.4153000e+00 -2.9459000e-02 /
CHEB / 2.3336000e+00 9.9855000e-01 -3.0438000e-02 /
CHEB / 4.2469000e-01 5.8732000e-01 2.6591000e-02 /
CHEB / -3.4207000e-01 1.5817000e-01 5.7246000e-02 /
CHEB / -3.0642000e-01 -1.0959000e-01 3.5134000e-02 /

CH3C[OH]CH3+C5H9J(9)(+m)=H2O+C8H14(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4513 (C8H16O(519))      deltaHrxn(T=298K) = -
71.85297968430174 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3937000e+00 -1.4371000e+00 -2.3563000e-02 /
CHEB / 3.2704000e+00 9.7576000e-01 -2.5099000e-02 /
CHEB / 4.7269000e-01 6.0581000e-01 2.0156000e-02 /
CHEB / -4.0043000e-01 1.9831000e-01 4.6556000e-02 /
CHEB / -3.6195000e-01 -8.4961000e-02 3.0715000e-02 /

HOC[CH2][CH3]2+iC4H7(+m)=H2O+C8H14(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4513 (C8H16O(519))      deltaHrxn(T=298K) = -
60.71418812163029 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5411000e+00 -1.4542000e+00 -1.8780000e-02 /
CHEB / 5.0410000e+00 9.5702000e-01 -2.0432000e-02 /
CHEB / 6.5939000e-01 6.1876000e-01 1.5246000e-02 /
CHEB / -4.1315000e-01 2.2995000e-01 3.7031000e-02 /
CHEB / -3.9467000e-01 -6.3262000e-02 2.5556000e-02 /

C4H8O-i1+iC4H8(+m)=H2O+C8H14(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4513 (C8H16O(519))     deltaHrxn(T=298K) = -
12.459111179136059 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3664000e+01 -1.4590000e+00 -1.7401000e-02 /
CHEB / 2.1783000e+01 9.5159000e-01 -1.9059000e-02 /
CHEB / 1.0201000e+00 6.2215000e-01 1.3844000e-02 /
CHEB / -3.1628000e-01 2.3882000e-01 3.4163000e-02 /
CHEB / -3.7140000e-01 -5.6852000e-02 2.3880000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
```

```
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+HOC[CH2][CH3]2(+m)=tSPC(97)+iC4H7(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4748 (C8H16O3(455))
      deltaHrxn(T=298K) = -14.23859049245631 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7946000e+00 -3.1237000e-01 -1.4990000e-01 /
CHEB / 1.9703000e+00 3.8581000e-01 1.7546000e-01 /
CHEB / 5.7961000e-01 -2.0876000e-02 4.7858000e-03 /
CHEB / 4.6431000e-02 -6.1342000e-02 -3.0512000e-02 /
CHEB / -4.1467000e-02 -6.6549000e-03 -8.6538000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+iC4H7(+m)=C4H7OJ(79)+CH3O(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C5H10O2(349))  deltaHrxn(T=298K) = -
18.727997366021764 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.3251000e+01 -1.7693000e-01 -1.0609000e-01 /
CHEB / -4.5503000e-01 2.1485000e-01 1.2621000e-01 /
CHEB / -2.9328000e-02 -5.1763000e-03 1.9642000e-04 /
CHEB / -1.9120000e-02 -3.6832000e-02 -2.1052000e-02 /
CHEB / -4.8366000e-03 -5.1016000e-03 -4.9631000e-03 /

tSPC(54)+CH3(+m)=C4H7OJ(79)+CH3O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C5H10O2(349))  deltaHrxn(T=298K) = -
30.976348487848963 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3294000e+01 -9.1388000e-03 -7.5767000e-03 /
CHEB / -1.2149000e-01 9.9803000e-03 8.2996000e-03 /
CHEB / 1.0181000e-02 2.0133000e-03 1.6168000e-03 /
CHEB / 4.6401000e-02 -3.1159000e-03 -2.5565000e-03 /
CHEB / 2.3325000e-02 -5.7472000e-04 -4.6380000e-04 /

tSPC(54)+CH3(+m)=sSPC(1697)+iC4H7(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C5H10O2(349))  deltaHrxn(T=298K) = -
12.248351121827199 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2329000e+00 -2.3602000e-02 -1.6255000e-02 /
CHEB / 1.7579000e+00 2.8285000e-02 1.9464000e-02 /
CHEB / 5.9263000e-01 -2.2427000e-04 -1.4619000e-04 /
CHEB / 1.8634000e-01 -5.1686000e-03 -3.5312000e-03 /
CHEB / 4.6305000e-02 -3.4391000e-04 -2.5894000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:
```

```
tSPC(122)+CH3(+m)=tSPC(77)+sSPC(1697)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (C5H10O4(431))  deltaHrxn(T=298K) = -
12.248351082962657 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0805000e+00 -6.5430000e-02 -4.2480000e-02 /
CHEB / 1.6413000e+00 8.4120000e-02 5.4194000e-02 /
CHEB / 5.5626000e-01 -9.5741000e-03 -5.5597000e-03 /
CHEB / 1.2528000e-01 -1.2497000e-02 -8.1646000e-03 /
CHEB / 1.4439000e-02 9.2129000e-04 3.1582000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(97)+CH3(+m)=sSPC(1697)+HOC[CH2][CH3]2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9 (C5H12O3(502)) deltaHrxn(T=298K)
= 1.9902393706291086 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3658000e+00 -4.8495000e-02 -3.1970000e-02 /
CHEB / 4.1984000e+00 5.5576000e-02 3.6270000e-02 /
CHEB / 8.7248000e-01 -4.6849000e-03 -2.8275000e-03 /
CHEB / 2.0237000e-01 -1.0411000e-02 -6.8242000e-03 /
CHEB / 2.4760000e-02 3.6791000e-04 9.9294000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1474)+H(+m)=H2CCCH3[OH]+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #18 (C3H7O3J(623)) deltaHrxn(T=298K) = -
18.917986764900743 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0275000e+01 -1.5826000e-01 -9.3634000e-02 /
CHEB / 1.2797000e+00 1.4841000e-01 8.4498000e-02 /
CHEB / -2.5819000e-01 1.3791000e-02 9.2560000e-03 /
CHEB / -2.2948000e-01 -2.0327000e-02 -1.0183000e-02 /
CHEB / -1.6155000e-01 -4.9233000e-03 -3.4342000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     tSPC(343)   -9.84 83.82 25.39 30.56 34.79 38.21 43.57 47.08 51.06
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!Here are the path reactions and their high-P limit kinetics:

O+tSPC(213)(+m)=tSPC(343)+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #24 (C4H6O4JJ(809))     deltaHrxn(T=298K) = -
23.357312578564287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5006000e+00 -7.7925000e-04 -5.4235000e-04 /
CHEB / 1.5756000e+00 9.4892000e-04 6.6044000e-04 /
CHEB / -5.1502000e-02 -8.5833000e-05 -5.9727000e-05 /
CHEB / -8.4004000e-02 -8.2539000e-05 -5.7446000e-05 /
CHEB / -7.0189000e-02 -1.2050000e-05 -8.3899000e-06 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(343)   -9.84 83.82 25.39 30.56 34.79 38.21 43.57 47.08 51.06
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(343)+CH3(+m)=C4H7OJ(79)+HCO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #94 (C5H8O2JJ(762))      deltaHrxn(T=298K) = -
0.8696208791862219 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0624000e+00 -1.0838000e-06 -7.5440000e-07 /
CHEB / 5.1966000e+00 3.6076000e-07 2.5111000e-07 /
CHEB / 3.5265000e-01 7.0968000e-07 4.9399000e-07 /
CHEB / 5.8728000e-02 1.5377000e-07 1.0704000e-07 /
CHEB / -2.6097000e-02 -8.0864000e-08 -5.6287000e-08 /

C4H7OJ(79)+HCO(+m)=CH2O+tSPC(110)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #94 (C5H8O2JJ(762))      deltaHrxn(T=298K) = -
23.97753330832302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0221000e+01 5.8760000e-09 4.0900000e-09 /
CHEB / 1.1032000e+00 2.1690000e-08 1.5098000e-08 /
CHEB / -8.6757000e-02 8.8817000e-09 6.1824000e-09 /
CHEB / -5.8284000e-02 1.1120000e-09 7.7395000e-10 /
CHEB / -5.2379000e-02 -2.2622000e-09 -1.5747000e-09 /

tSPC(343)+CH3(+m)=CH2O+tSPC(110)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #94 (C5H8O2JJ(762))      deltaHrxn(T=298K) = -
24.84715418750925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9378000e+00 1.3321000e-08 9.2725000e-09 /
CHEB / 3.0525000e+00 2.2321000e-08 1.5537000e-08 /
CHEB / -8.0299000e-02 1.2079000e-08 8.4081000e-09 /
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CHEB / -3.4848000e-02 1.9159000e-09 1.3336000e-09 /
CHEB / -3.6654000e-02 -4.4470000e-09 -3.0954000e-09 /

!PDepNetwork tSPC(343)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(343)   -6.43 80.94 25.61 31.29 35.94 39.68 45.17 48.86 53.87
!MRH CBS-QB3 w/1DHR corrections
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CH2CHCH2O   25.06 72.63 18.45 22.37 25.85 28.76 33.26 36.56 41.63
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     iC4H5OJ(15) 12.77 74.84 22.08 26.8  30.77 34.04 39.05 42.66 48.02
!MRH CBS-QB3 w/1DHR corrections
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+tSPC(346)=tSPC(343)      3.2847733e+07      1.50370
7.3354000e+03
!     CH2CHCH2O+CO=tSPC(343)  5.9198482e+04      2.36750
7.2970000e+04
!     O+iC4H5OJ(15)=tSPC(343) 1.0000000e+13      0.00000
0.0000000e+00

CH2O+tSPC(346)(+m)=tSPC(343)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(343)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H2_O     Cd_rad/OneDe         deltaHrxn(T=298K)
= -26.65738314257927 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3551000e+00 1.1005000e+00 -1.7398000e-01 /
CHEB / 1.2594000e+00 7.7408000e-01 1.2214000e-01 /
CHEB / -6.7137000e-01 1.9869000e-01 5.0092000e-02 /
CHEB / -1.7504000e-01 -3.4825000e-02 7.4883000e-03 /
CHEB / -2.6775000e-02 -3.4179000e-02 -4.8633000e-03 /

tSPC(343)(+m)=CH2CHCH2O+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(343))    deltaHrxn(T=298K) = 5.049485153069689
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1334000e+01 1.9996000e+00 -2.9610000e-04 /
CHEB / 2.5943000e+01 2.3261000e-04 1.6186000e-04 /
CHEB / -1.7521000e-01 5.4142000e-05 3.7675000e-05 /
CHEB / 1.6118000e-02 -5.4544000e-05 -3.7947000e-05 /
CHEB / 4.4207000e-03 -6.3117000e-06 -4.3925000e-06 /
```

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CH2O+tSPC(346)(+m)=CH2CHCH2O+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(343))    deltaHrxn(T=298K) = -21.60789798950958
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.6846000e+00 -3.8139000e-04 -2.6541000e-04 /
CHEB / 1.8165000e+01 2.6719000e-04 1.8592000e-04 /
CHEB / 3.0739000e-01 4.8920000e-05 3.4041000e-05 /
CHEB / 1.1448000e-01 -5.6494000e-05 -3.9306000e-05 /
CHEB / 3.6933000e-02 -6.9660000e-06 -4.8485000e-06 /

O+iC4H5OJ(15)(+m)=tSPC(343)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(343)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Oa     C_rad/H2/Cd       deltaHrxn(T=298K) = -
78.83183466271647 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8512000e+00 1.9996000e+00 -2.9610000e-04 /
CHEB / -7.9390000e-01 2.3261000e-04 1.6186000e-04 /
CHEB / -1.1672000e-01 5.4142000e-05 3.7675000e-05 /
CHEB / 4.7072000e-02 -5.4544000e-05 -3.7947000e-05 /
CHEB / 1.3946000e-02 -6.3117000e-06 -4.3925000e-06 /

O+iC4H5OJ(15)(+m)=CH2O+tSPC(346)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5 (tSPC(343))     deltaHrxn(T=298K) = -
52.174451520137204 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3514000e+01 -3.8139000e-04 -2.6541000e-04 /
CHEB / -4.1948000e-01 2.6719000e-04 1.8592000e-04 /
CHEB / -5.1207000e-03 4.8920000e-05 3.4041000e-05 /
CHEB / 7.8222000e-03 -5.6494000e-05 -3.9306000e-05 /
CHEB / -1.0175000e-04 -6.9660000e-06 -4.8485000e-06 /

O+iC4H5OJ(15)(+m)=CH2CHCH2O+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(343))    deltaHrxn(T=298K) = -73.78234950964678
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5864000e+00 -2.1877000e-04 -1.5226000e-04 /
CHEB / 3.6368000e+00 1.9290000e-04 1.3425000e-04 /
CHEB / 9.2419000e-01 -1.0420000e-05 -7.2473000e-06 /
CHEB / 2.3496000e-01 -2.9153000e-05 -2.0289000e-05 /
CHEB / 7.6357000e-02 -3.0552000e-06 -2.1275000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     tSPC(157)   -4.85 104.09      37.36 44.83 50.46 55.08 61.65 66.34
      72.86 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(157)+CH2O(+m)=tSPC(77)+sSPC(3121)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #187 (C5H9O5J(1559))
      deltaHrxn(T=298K) = -26.777083813918573 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.5642000e+00 -2.6361000e-02 -1.7877000e-02 /
CHEB / 1.5579000e+01 3.8892000e-02 2.6284000e-02 /
CHEB / 5.1126000e-02 -1.3510000e-02 -8.9624000e-03 /
CHEB / -8.2956000e-02 -3.0658000e-04 -3.5251000e-04 /
CHEB / -1.1487000e-02 1.4794000e-03 1.0292000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H6O(105)  -2.12 71.03 19.46 26.19 31.81 36.09 42.58 47.31 53.93
      null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!Here are the path reactions and their high-P limit kinetics:

C4H6O(105)+H2O(+m)=H2CCCH3[OH]+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #209 (C4H8O2(994)) deltaHrxn(T=298K) = -
4.839745015520247 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2217000e+01 -1.2151000e+00 -6.1047000e-02 /
CHEB / 2.0596000e+01 1.1161000e+00 -2.3728000e-02 /
CHEB / 2.2103000e-01 3.3458000e-01 7.5332000e-02 /
CHEB / -1.3487000e-01 -9.6201000e-02 4.8845000e-02 /
CHEB / -2.4655000e-02 -1.3675000e-01 -1.0516000e-02 /

!PDepNetwork
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```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H2CCCO      33.02 66.05 15.09 17.26 19.13 20.72 23.23 25.1  27.95
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+tSPC(346)=tSPC(878)  1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(878)=HO2+H2CCCO    5.8013126e+10      0.62333
3.0055556e+04

O2+tSPC(346)(+m)=tSPC(878)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(878)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     Cd_rad/OneDe      deltaHrxn(T=298K) = -
45.19553276273392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7954000e+00 3.3796000e+00 -5.9170000e-01 /
CHEB / -4.3803000e+00 1.2353000e+00 3.6357000e-01 /
CHEB / -2.3408000e+00 2.6430000e-01 1.7380000e-01 /
CHEB / -1.1864000e+00 -7.3980000e-02 4.3923000e-02 /
CHEB / -5.5375000e-01 -1.0921000e-01 -7.3123000e-03 /

H2CCCO+HO2(+m)=tSPC(878)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(878))    deltaHrxn(T=298K) = -34.15664106789909
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0580000e+01 6.5323000e-01 -5.4300000e-02 /
CHEB / -3.8518000e+00 9.9150000e-01 -3.5042000e-02 /
CHEB / -1.5588000e+00 4.2509000e-01 4.4464000e-02 /
CHEB / -9.7148000e-01 3.6787000e-02 4.3752000e-02 /
CHEB / -4.9419000e-01 -9.3948000e-02 6.4005000e-03 /

O2+tSPC(346)(+m)=H2CCCO+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(878))    deltaHrxn(T=298K) = -11.038891694834831
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 1.2158000e+01 -3.1138000e-01 -1.6828000e-01 /
CHEB / -4.1355000e-02 3.7645000e-01 1.9185000e-01 /
CHEB / -8.3741000e-02 -1.3365000e-02 8.9121000e-03 /
CHEB / -6.3612000e-02 -5.3255000e-02 -2.8429000e-02 /
CHEB / -2.3126000e-02 -1.0716000e-02 -1.0749000e-02 /

!PDepNetwork tSPC(1286)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1286)  -11.0 79.85 22.68 26.88 30.42 33.26 37.32 39.96 43.51
!MRH CBS-QB3 w/1DHR corrections
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     H2CCCO      33.02 66.05 15.09 17.26 19.13 20.72 23.23 25.1  27.95
!     tSPC(1553)  -19.27      73.08 18.28 22.22 25.51 28.12 31.86 34.37
      37.97  !MRH CBS-QB3 w/1DHR corrections
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+C3H3O-enone=tSPC(1286)     1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(1286)=HO2+H2CCCO   5.800e+10    0.62        45000.00
!     tSPC(1553)+O=tSPC(1286) 1.0000000e+13      0.00000
0.0000000e+00

O2+C3H3O-enone(+m)=tSPC(1286)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     CO_rad/OneDe      deltaHrxn(T=298K) = -
36.19634590414202 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1375000e+01 1.0598000e+00 -1.7950000e-01 /
CHEB / -1.4851000e+00 7.0791000e-01 1.0393000e-01 /
CHEB / -7.3478000e-01 2.2405000e-01 4.9324000e-02 /
CHEB / -2.2697000e-01 5.7651000e-03 1.3605000e-02 /
CHEB / -3.6329000e-02 -2.5555000e-02 -2.0686000e-03 /

HO2+H2CCCO(+m)=tSPC(1286)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286))   deltaHrxn(T=298K) = -47.08512923916946
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1708000e+00 1.7915000e+00 -1.1854000e-01 /
CHEB / -8.8290000e-01 1.7520000e-01 9.7738000e-02 /
CHEB / -1.4293000e-01 4.7228000e-02 2.6384000e-02 /
CHEB / 4.2937000e-02 -1.5191000e-02 -6.9313000e-03 /
CHEB / 7.2992000e-02 -1.2178000e-02 -6.4713000e-03 /
```

```
O2+C3H3O-enone(+m)=HO2+H2CCCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286))   deltaHrxn(T=298K) = 10.888783335027437
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1187000e+00 -1.5218000e-01 -8.8170000e-02 /
CHEB / 4.0190000e+00 1.6847000e-01 9.6007000e-02 /
CHEB / 3.2041000e-01 8.5479000e-03 5.9953000e-03 /
CHEB / 9.7425000e-02 -2.5410000e-02 -1.3637000e-02 /
CHEB / 3.3282000e-02 -6.5870000e-03 -4.2366000e-03 /

tSPC(1553)+O(+m)=tSPC(1286)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/OneDe     Oa       deltaHrxn(T=298K) = -
51.364759794927025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0261000e+01 1.9505000e+00 -3.3056000e-02 /
CHEB / -9.6711000e-01 4.0003000e-02 2.6643000e-02 /
CHEB / -3.8634000e-01 1.2378000e-02 8.1746000e-03 /
CHEB / -4.3083000e-02 -5.1950000e-03 -3.3403000e-03 /
CHEB / 3.7761000e-02 -3.6165000e-03 -2.3695000e-03 /

tSPC(1553)+O(+m)=O2+C3H3O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286))   deltaHrxn(T=298K) = -15.168413890785
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3077000e+01 -3.9428000e-02 -2.6414000e-02 /
CHEB / -7.3162000e-02 4.0347000e-02 2.6947000e-02 /
CHEB / -9.1514000e-03 5.7091000e-03 3.8151000e-03 /
CHEB / -6.9649000e-03 -7.0248000e-03 -4.6006000e-03 /
CHEB / -5.9740000e-03 -2.4445000e-03 -1.6439000e-03 /

tSPC(1553)+O(+m)=HO2+H2CCCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (tSPC(1286))   deltaHrxn(T=298K) = -4.279630555757564
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3587000e+00 -3.3458000e-02 -2.2484000e-02 /
CHEB / 1.9425000e+00 3.6865000e-02 2.4690000e-02 /
CHEB / 5.5126000e-01 1.8242000e-03 1.2616000e-03 /
CHEB / 1.6037000e-01 -6.3333000e-03 -4.1827000e-03 /
CHEB / 4.8541000e-02 -1.1738000e-03 -8.1755000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H3O-enone=C4H6O(717)    1.4157154e+13      -0.15000
2.9166667e+02
!     CH3CO+C2H3=C4H6O(717)   1.4157154e+13      -0.15000
2.9166667e+02
!     C3H6+CO=C4H6O(717)      5.3800000e+02      3.29000
1.0450000e+05

CH3CO+C2H3(+m)=C4H6O(717)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #636 (C4H6O(717)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/NonDe     Cd_pri_rad          deltaHrxn(T=298K) = -
99.72973367720928 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1912000e+01 1.1512000e+00 -2.4044000e-01 /
CHEB / -1.6429000e+00 6.4834000e-01 1.3025000e-01 /
CHEB / -7.4449000e-01 2.4165000e-01 8.4410000e-02 /
CHEB / -2.9275000e-01 7.3652000e-03 3.1473000e-02 /
CHEB / -7.9003000e-02 -4.5578000e-02 -3.6784000e-03 /

CH3CO+C2H3(+m)=CH3+C3H3O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #636 (C4H6O(717)) deltaHrxn(T=298K) = -23.94808423731211
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2579000e+01 -7.5349000e-01 -2.2022000e-01 /
CHEB / 1.2766000e-01 6.9873000e-01 1.5974000e-01 /
CHEB / 7.7179000e-02 1.7248000e-01 8.2990000e-02 /
CHEB / -4.0978000e-02 -5.1413000e-02 1.0676000e-02 /
CHEB / -3.5869000e-02 -5.9438000e-02 -2.0048000e-02 /

C4H6O(717)(+m)=C3H6+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #636 (C4H6O(717)) deltaHrxn(T=298K) = 8.62886870948693
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3412000e+01 1.6019000e+00 -1.9426000e-01 /
CHEB / 3.7795000e+01 3.3995000e-01 1.5357000e-01 /
CHEB / -5.3428000e-01 1.0526000e-01 5.6639000e-02 /
CHEB / -2.1406000e-01 -1.8009000e-02 -9.1502000e-04 /
CHEB / -3.7937000e-02 -3.0012000e-02 -1.3494000e-02 /

CH3+C3H3O-enone(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #636 (C4H6O(717)) deltaHrxn(T=298K) = -67.15278073041024
kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6884000e+00 -3.6384000e-01 -1.7872000e-01 /
CHEB / 1.3740000e+01 3.5250000e-01 1.6264000e-01 /
CHEB / 3.2284000e-01 7.5535000e-02 4.5093000e-02 /
CHEB / 1.2665000e-01 -3.7076000e-02 -1.1693000e-02 /
CHEB / 5.3308000e-02 -3.0036000e-02 -1.6029000e-02 /

CH3CO+C2H3(+m)=C3H6+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #636 (C4H6O(717)) deltaHrxn(T=298K) = -91.10086496772236
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8668000e+00 -3.2596000e-01 -1.6282000e-01 /
CHEB / 6.7566000e+00 3.4693000e-01 1.6352000e-01 /
CHEB / 7.7717000e-01 3.7923000e-02 2.9074000e-02 /
CHEB / 2.1668000e-01 -4.4838000e-02 -1.8391000e-02 /
CHEB / 6.9918000e-02 -2.1671000e-02 -1.3892000e-02 /

!PDepNetwork C3H3O-enone && C3H3OJ && tSPC(346)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!     C3H3OJ      41.87 70.08 16.16 18.35 20.4  22.25 25.39 27.81 31.6
      null
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     CHCHCHO     45.67 67.33 16.24 19.74 22.69 25.03 28.29 30.37 33.17
!     H2CCCO      33.02 66.05 15.09 17.26 19.13 20.72 23.23 25.1  27.95
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2O               75.16 57.47 12.08 13.91 15.4  16.64 18.61 20.1
      22.47 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HCCCHO      33.48 65.54 15.1  17.48 19.41 20.99 23.45 25.24 27.98
!     pC3H3             86.21 60.63 14.9  17.21 19.0  20.43 22.68 24.42
      27.32
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     H2CCCO+H=C3H3O-enone    1.2000000e+11      0.69000
3.0000000e+03
!     C3H3OJ=C3H3O-enone      1.8288499e+09      1.13906
3.4790987e+04
!     H2CCCO+H=C3H3OJ         6.6800000e+13      0.00000
2.9000000e+03
!     CH3+C2O=C3H3OJ          1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(346)=C3H3O-enone   2.0320555e+08      1.13906
3.4790987e+04
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!     HCCCHO+H=tSPC(346)      1.8600000e+13      0.00000
2.3000000e+03
!     H2CCCO+H=tSPC(346)      5.2263889e+12      0.04600
5.0666667e+03
!     CHCHCHO=tSPC(346)       1.9697990e+11      0.77000
4.5050000e+04
!     O+pC3H3=tSPC(346)       1.0000000e+13      0.00000
0.0000000e+00
!     CHCHCHO=C3H3O-enone     2.0320555e+08      1.13906
3.4790987e+04
!     C2H3+CO=C3H3O-enone     1.5100000e+11      0.00000
4.8100000e+03

C3H3OJ(+m)=C3H3O-enone(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    Y_rad_out     Cs_H_out_2H
      deltaHrxn(T=298K) = -17.351129265431727 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5859000e+01 8.0088000e+00 2.1535000e-01 /
CHEB / 1.0754000e+01 5.5516000e-02 -1.1879000e-01 /
CHEB / -9.6067000e-01 -4.6840000e-01 1.3580000e-01 /
CHEB / -7.2182000e-01 -1.6156000e-01 1.0417000e-01 /
CHEB / -5.4295000e-01 9.8248000e-02 3.6682000e-02 /

tSPC(346)(+m)=C3H3O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    Cd_rad_out_double     CO_H_out
      deltaHrxn(T=298K) = -21.927675029862268 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7888000e+01 6.8131000e+00 1.0828000e+00 /
CHEB / 1.1738000e+01 -2.2519000e-01 -4.4231000e-01 /
CHEB / -5.0003000e-01 -4.9933000e-01 -9.7424000e-02 /
CHEB / -4.5236000e-01 -2.9844000e-01 1.2515000e-01 /
CHEB / -3.8125000e-01 -9.8496000e-02 1.7555000e-01 /

tSPC(346)(+m)=C3H3OJ(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -4.576545764430541
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1953000e+01 3.4500000e+00 -6.4471000e-01 /
CHEB / 1.0630000e+01 1.7839000e+00 4.3801000e-01 /
CHEB / -1.4128000e+00 2.6296000e-01 2.5375000e-01 /
CHEB / -8.6826000e-01 -1.0161000e-01 4.2102000e-02 /
CHEB / -4.4041000e-01 -1.0982000e-01 -2.9497000e-02 /

H2CCCO+H(+m)=C3H3O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: R_Addition_MultipleBond
exact:  Ca_Cd/H2     H_rad          deltaHrxn(T=298K) = -
60.59321221549314 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.5641000e+00 7.3718000e+00 7.2091000e-01 /
CHEB / 9.2619000e-01 1.3564000e-01 2.3237000e-01 /
CHEB / -4.3391000e-01 -6.6192000e-01 7.9472000e-02 /
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CHEB / -3.0015000e-01 -5.4643000e-01 9.5582000e-02 /
CHEB / -2.1455000e-01 -2.8963000e-01 1.1966000e-01 /

H2CCCO+H(+m)=C3H3OJ(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone) High-P Limit: R_Addition_MultipleBond exact:  Cd/H2_Ca
H_rad       deltaHrxn(T=298K) = -43.242082950061416 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1176000e+00 4.3226000e+00 -7.6748000e-01 /
CHEB / -2.4854000e+00 1.0977000e+00 7.2265000e-01 /
CHEB / -1.6362000e+00 -7.5210000e-02 3.4063000e-01 /
CHEB / -7.8472000e-01 -1.6599000e-01 6.3409000e-02 /
CHEB / -3.8130000e-01 -6.9019000e-02 -3.6786000e-02 /

H2CCCO+H(+m)=tSPC(346)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_Ca     H_rad      deltaHrxn(T=298K) = -
38.665537185630875 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3940000e+00 1.2780000e+00 -3.0067000e-01 /
CHEB / -6.5384000e-01 1.4097000e+00 -1.0110000e-01 /
CHEB / -1.3554000e+00 5.2270000e-01 6.5482000e-02 /
CHEB / -7.0711000e-01 1.0455000e-01 5.4476000e-02 /
CHEB / -3.5049000e-01 -2.4391000e-02 1.6993000e-02 /

CH3+C2O(+m)=C3H3O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -85.88048658530393
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0084000e+01 1.0912000e+01 1.6959000e+00 /
CHEB / -1.7170000e+00 -7.2610000e-01 3.3325000e-01 /
CHEB / -1.0119000e+00 -8.0848000e-01 -3.3443000e-01 /
CHEB / -4.9815000e-01 -5.1127000e-01 -1.5230000e-01 /
CHEB / -2.5740000e-01 -2.9105000e-01 3.8858000e-02 /

CH3+C2O(+m)=C3H3OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone) High-P Limit: R_Recombination estimate: (Average:)
C_methyl     Ct_rad           deltaHrxn(T=298K) = -68.5293573198722
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7269000e+00 9.3496000e+00 -5.7326000e-01 /
CHEB / -4.5024000e+00 -7.9639000e-01 1.2846000e+00 /
CHEB / -1.5526000e+00 -1.2599000e+00 3.6465000e-01 /
CHEB / -7.1713000e-01 -5.6560000e-01 4.8992000e-02 /
CHEB / -4.2536000e-01 -9.6299000e-02 -3.8529000e-02 /

CH3+C2O(+m)=tSPC(346)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -63.95281155544166
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6366000e-01 5.5224000e+00 -7.4173000e-01 /
CHEB / -1.5020000e+00 8.6397000e-01 7.7191000e-01 /
CHEB / -1.1787000e+00 -9.3081000e-02 2.8100000e-01 /
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CHEB / -6.9074000e-01 -1.1695000e-01 7.0179000e-02 /
CHEB / -3.8811000e-01 -1.2249000e-02 -1.5478000e-02 /

H2CCCO+H(+m)=CH3+C2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = 25.28727436981078
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3325000e+00 -8.1760000e-02 -5.6695000e-02 /
CHEB / 8.9751000e+00 1.0942000e-01 7.5024000e-02 /
CHEB / 1.3912000e-01 -2.2341000e-02 -1.3754000e-02 /
CHEB / 2.2624000e-02 -8.1641000e-03 -6.6835000e-03 /
CHEB / -1.0924000e-02 1.3997000e-03 9.4329000e-04 /

HCCCHO+H(+m)=C3H3O-enone(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -61.053178577514174
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.7085000e+00 5.6051000e+00 1.0253000e+00 /
CHEB / 1.7838000e+00 8.7136000e-01 -5.7279000e-01 /
CHEB / -1.5086000e-01 -1.3395000e-01 -4.5851000e-02 /
CHEB / -3.2591000e-01 -2.9095000e-01 1.9517000e-01 /
CHEB / -3.2970000e-01 -1.8126000e-01 2.1500000e-01 /

HCCCHO+H(+m)=C3H3OJ(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -43.70204931208245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2767000e+00 3.1350000e+00 -7.6387000e-01 /
CHEB / 7.4903000e-02 2.2184000e+00 6.0865000e-01 /
CHEB / -1.2094000e+00 2.5581000e-01 2.7770000e-01 /
CHEB / -7.3813000e-01 -1.3018000e-01 5.7732000e-02 /
CHEB / -3.6518000e-01 -9.4566000e-02 -9.6032000e-03 /

HCCCHO+H(+m)=tSPC(346)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: R_Addition_MultipleBond
exact:  Ct/H_Ct/De     H_rad        deltaHrxn(T=298K) = -
39.12550354765191 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1185000e+01 9.6017000e-01 -1.9425000e-01 /
CHEB / -1.3459000e+00 1.2670000e+00 -1.2468000e-01 /
CHEB / -1.2869000e+00 5.2758000e-01 3.6053000e-02 /
CHEB / -6.8748000e-01 1.2182000e-01 4.7266000e-02 /
CHEB / -3.4497000e-01 -1.7849000e-02 1.6677000e-02 /

HCCCHO+H(+m)=H2CCCO+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -0.459966362021035
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0261000e+01 -9.0167000e-01 -1.5985000e-01 /
CHEB / 2.2216000e+00 9.3811000e-01 9.0383000e-02 /
CHEB / -1.7171000e-02 1.0805000e-01 1.0152000e-01 /
CHEB / -7.3234000e-02 -8.9635000e-02 5.9236000e-03 /
CHEB / -2.6971000e-02 -5.6670000e-02 -2.6023000e-02 /
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HCCCHO+H(+m)=CH3+C2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = 24.827308007789746
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1350000e+00 -2.7022000e-01 -1.7821000e-01 /
CHEB / 1.0805000e+01 3.4416000e-01 2.2080000e-01 /
CHEB / 6.1366000e-01 -4.3597000e-02 -1.8649000e-02 /
CHEB / 1.5370000e-01 -3.6056000e-02 -2.6312000e-02 /
CHEB / 2.9185000e-02 -1.9588000e-03 -3.4085000e-03 /

O+pC3H3(+m)=C3H3O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -121.3171528070137
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1699000e+01 1.4221000e+01 3.6319000e+00 /
CHEB / -1.3054000e+00 -9.6558000e-01 -9.9146000e-01 /
CHEB / -7.9006000e-01 -6.0332000e-01 -7.4917000e-01 /
CHEB / -5.0103000e-01 -4.0884000e-01 -1.7527000e-01 /
CHEB / -3.7803000e-01 -2.8675000e-01 1.4226000e-01 /

O+pC3H3(+m)=C3H3OJ(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -103.96602354158198 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5481000e+01 1.5172000e+01 1.5724000e+00 /
CHEB / -2.7011000e+00 -2.5782000e+00 2.2757000e-01 /
CHEB / -1.1590000e+00 -1.1541000e+00 -3.4216000e-01 /
CHEB / -6.0042000e-01 -5.3042000e-01 -6.7244000e-02 /
CHEB / -3.4491000e-01 -2.8850000e-01 1.0644000e-01 /

O+pC3H3(+m)=tSPC(346)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: Oa_R_Recombination estimate:
(Average:) Oa     Cd_pri_rad        deltaHrxn(T=298K) = -
99.38947777715143 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9254000e+00 1.2947000e+01 1.0119000e+00 /
CHEB / -3.2949000e+00 -2.3108000e+00 -1.3089000e-02 /
CHEB / -1.0690000e+00 -1.2406000e+00 -3.0055000e-01 /
CHEB / -5.4809000e-01 -5.3764000e-01 1.0490000e-02 /
CHEB / -4.2218000e-01 -1.6014000e-01 1.7901000e-01 /

O+pC3H3(+m)=H2CCCO+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -60.72394059152057
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2477000e+01 -3.6083000e-04 -2.5626000e-04 /
CHEB / -1.5487000e-01 4.1847000e-04 2.9874000e-04 /
CHEB / -3.3138000e-02 -2.7475000e-05 -2.1794000e-05 /
CHEB / 1.2145000e-02 -2.2416000e-05 -1.5331000e-05 /
CHEB / 8.5084000e-03 -9.9837000e-06 -6.9283000e-06 /
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O+pC3H3(+m)=CH3+C2O(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -35.43666622170977 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1859000e+00 -1.0192000e-02 -7.1581000e-03 /
CHEB / 2.6405000e+00 1.2560000e-02 8.8369000e-03 /
CHEB / 5.3402000e-01 -1.6149000e-03 -1.1572000e-03 /
CHEB / 1.2068000e-01 -6.9843000e-04 -4.8448000e-04 /
CHEB / 8.7509000e-03 -1.3081000e-04 -8.9689000e-05 /

O+pC3H3(+m)=HCCCHO+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -60.26397422949953
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2918000e+01 1.1074000e-04 7.6844000e-05 /
CHEB / -1.6292000e-01 -1.1720000e-04 -8.0926000e-05 /
CHEB / -4.5522000e-02 -4.8833000e-07 -1.0842000e-06 /
CHEB / 4.3004000e-03 7.2032000e-06 5.4377000e-06 /
CHEB / 4.1418000e-03 -4.8016000e-07 -4.0955000e-07 /

C2H3+CO(+m)=C3H3O-enone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone) High-P Limit: R_Addition_COm exact:
Cd_pri_rad     COm      deltaHrxn(T=298K) = -21.2375821754618 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3456000e+00 1.3826000e+00 -1.9674000e-01 /
CHEB / -5.8490000e-01 4.9790000e-01 1.6411000e-01 /
CHEB / -1.2052000e+00 1.5219000e-01 4.5626000e-02 /
CHEB / -5.7198000e-01 1.6932000e-03 9.5446000e-04 /
CHEB / -2.5844000e-01 -2.5859000e-02 -7.7454000e-03 /

C3H3OJ(+m)=C2H3+CO(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = 3.8864529100300764 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.1319000e+00 1.9830000e+00 -4.7663000e-01 /
CHEB / 9.6348000e+00 1.3920000e+00 1.3647000e-01 /
CHEB / -1.3596000e+00 3.1396000e-01 1.8384000e-01 /
CHEB / -7.2202000e-01 -2.7308000e-02 6.4622000e-02 /
CHEB / -3.4771000e-01 -8.1443000e-02 -1.8111000e-03 /

tSPC(346)(+m)=C2H3+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -0.690092854400465
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6383000e+00 4.8540000e-01 -5.1738000e-02 /
CHEB / 1.0879000e+01 7.9398000e-01 -5.7655000e-02 /
CHEB / -9.2178000e-01 4.3565000e-01 1.1516000e-02 /
CHEB / -6.0022000e-01 1.4012000e-01 3.6246000e-02 /
CHEB / -3.2941000e-01 -4.3570000e-03 2.2020000e-02 /

H2CCCO+H(+m)=C2H3+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -39.35563004003134
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.1980000e+01 -6.9806000e-02 -2.1326000e-02 /
CHEB / 1.3670000e+00 6.6359000e-02 1.2093000e-02 /
CHEB / 6.8456000e-02 1.5820000e-02 1.4075000e-02 /
CHEB / 1.8720000e-02 -4.0937000e-03 1.0844000e-03 /
CHEB / -1.7857000e-03 -7.9343000e-03 -4.3654000e-03 /

CH3+C2O(+m)=C2H3+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -64.64290440984213 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1674000e+01 -4.9667000e-02 -3.9694000e-02 /
CHEB / -1.1057000e-02 7.2149000e-02 5.6900000e-02 /
CHEB / -1.4739000e-01 -2.1613000e-02 -1.5780000e-02 /
CHEB / -1.2171000e-01 -4.0840000e-03 -4.1467000e-03 /
CHEB / -8.3352000e-02 2.5244000e-03 2.0600000e-03 /

HCCCHO+H(+m)=C2H3+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -39.81559640205238
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0579000e+01 -1.0848000e+00 -1.1933000e-01 /
CHEB / 1.6171000e+00 1.0288000e+00 2.2393000e-02 /
CHEB / -2.7513000e-02 2.2485000e-01 1.0258000e-01 /
CHEB / -8.8948000e-02 -7.0992000e-02 3.5033000e-02 /
CHEB / -3.8745000e-02 -7.9035000e-02 -1.5718000e-02 /

O+pC3H3(+m)=C2H3+CO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -100.0795706315519 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1189000e+01 1.3502000e-03 9.5486000e-04 /
CHEB / 2.7604000e-01 -1.4835000e-03 -1.0533000e-03 /
CHEB / -6.2385000e-03 7.4571000e-05 5.7360000e-05 /
CHEB / -2.3673000e-02 7.9627000e-05 5.6190000e-05 /
CHEB / -3.0979000e-02 2.2405000e-05 1.5233000e-05 /

C3H3O-enone(+m)=CHCHCHO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = 21.14779750425811
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6066000e+01 6.6725000e+00 1.0390000e+00 /
CHEB / 1.9318000e+01 -5.0318000e-01 -3.3079000e-01 /
CHEB / -2.1561000e-01 -6.2303000e-01 -5.2836000e-02 /
CHEB / -2.8651000e-01 -3.0829000e-01 1.1974000e-01 /
CHEB / -2.8899000e-01 -6.3944000e-02 1.5714000e-01 /

C3H3OJ(+m)=CHCHCHO(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = 3.796668238826385 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3689000e+01 3.1778000e+00 -5.6294000e-01 /
CHEB / 1.2686000e+01 1.6765000e+00 4.7210000e-01 /
CHEB / -9.6274000e-01 1.8932000e-01 2.9230000e-01 /
CHEB / -6.1768000e-01 -1.2737000e-01 6.2223000e-02 /
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CHEB / -3.1085000e-01 -1.0224000e-01 -2.1519000e-02 /

tSPC(346)(+m)=CHCHCHO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -0.7798775256041566
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9411000e+00 1.3726000e+00 -3.3164000e-01 /
CHEB / 1.3121000e+01 1.4344000e+00 -8.6983000e-02 /
CHEB / -1.2380000e+00 5.1712000e-01 7.4148000e-02 /
CHEB / -6.9188000e-01 9.9231000e-02 5.6216000e-02 /
CHEB / -3.5003000e-01 -2.6270000e-02 1.7042000e-02 /

H2CCCO+H(+m)=CHCHCHO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -39.44541471123503
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4166000e+00 -8.2907000e-01 -1.7129000e-01 /
CHEB / 3.5250000e+00 8.8394000e-01 1.1377000e-01 /
CHEB / 2.1900000e-01 7.6779000e-02 9.5470000e-02 /
CHEB / 9.4915000e-03 -8.8634000e-02 -3.8653000e-03 /
CHEB / 6.2513000e-03 -4.8429000e-02 -2.6389000e-02 /

CH3+C2O(+m)=CHCHCHO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -64.73268908104582 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3766000e+00 -9.7576000e-02 -6.4966000e-02 /
CHEB / 2.1772000e+00 1.2513000e-01 8.2074000e-02 /
CHEB / 5.3779000e-01 -1.9336000e-02 -1.0749000e-02 /
CHEB / 1.1933000e-01 -9.8331000e-03 -7.3607000e-03 /
CHEB / 5.0558000e-04 -7.6674000e-05 -2.1593000e-04 /

HCCCHO+H(+m)=CHCHCHO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3O-enone)  deltaHrxn(T=298K) = -39.905381073256066
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5502000e+00 -8.7614000e-01 -1.6704000e-01 /
CHEB / 3.0314000e+00 9.1585000e-01 1.0198000e-01 /
CHEB / 1.6087000e-01 1.0070000e-01 9.8917000e-02 /
CHEB / -8.7815000e-03 -8.8393000e-02 3.0996000e-03 /
CHEB / -3.1083000e-03 -5.4670000e-02 -2.6103000e-02 /

O+pC3H3(+m)=CHCHCHO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -100.16935530275559 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1906000e+01 -4.8038000e-04 -3.4066000e-04 /
CHEB / 5.3033000e-01 5.5551000e-04 3.9578000e-04 /
CHEB / 1.4544000e-01 -3.4347000e-05 -2.7045000e-05 /
CHEB / 7.3144000e-02 -3.0457000e-05 -2.0967000e-05 /
CHEB / 3.1486000e-02 -1.2782000e-05 -8.8513000e-06 /

C2H3+CO(+m)=CHCHCHO(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7 (C3H3O-enone)  deltaHrxn(T=298K) = -0.08978467120368805 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6468000e+00 -1.6548000e-03 -7.4142000e-04 /
CHEB / 1.3074000e+01 -2.0571000e-03 -1.0445000e-03 /
CHEB / 4.6748000e-01 5.3848000e-04 -4.4707000e-05 /
CHEB / 1.9938000e-01 2.2815000e-03 8.3999000e-04 /
CHEB / 8.0681000e-02 2.0646000e-03 1.0729000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+H(+m)=tSPC(346)+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2037 (C3H4O3(1458))    deltaHrxn(T=298K) = -
23.117196974444326 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9339000e+00 -5.8517000e-06 -4.0732000e-06 /
CHEB / 1.1298000e+00 2.5319000e-06 1.7624000e-06 /
CHEB / 5.0028000e-01 1.3799000e-06 9.6053000e-07 /
CHEB / 2.2201000e-01 -5.4711000e-07 -3.8083000e-07 /
CHEB / 8.9611000e-02 -8.0034000e-07 -5.5710000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
```

```
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+tSPC(346)(+m)=tSPC(878)+iC4H7(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H10O3(412)) deltaHrxn(T=298K)
= -23.357533042895653 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6339000e+00 -4.4048000e-05 -3.0660000e-05 /
CHEB / 3.2136000e+00 3.8780000e-05 2.6993000e-05 /
CHEB / 1.0216000e+00 1.2564000e-05 8.7454000e-06 /
CHEB / 2.1367000e-01 -5.6069000e-06 -3.9026000e-06 /
CHEB / 9.4377000e-03 -3.0485000e-06 -2.1219000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+tSPC(54)(+m)=tSPC(1553)+C4H7OJ(79)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2593 (C7H10O3(2223))
      deltaHrxn(T=298K) = -38.635744203985304 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2732000e+01 -4.4825000e-02 -3.4882000e-02 /
```

```
CHEB / 2.7537000e-02 4.5545000e-02 3.5564000e-02 /
CHEB / 1.4827000e-02 1.2940000e-02 9.6725000e-03 /
CHEB / 2.3139000e-02 -1.1534000e-02 -8.6374000e-03 /
CHEB / 5.8384000e-03 -6.0379000e-03 -4.6019000e-03 /

C3H3O-enone+tSPC(54)(+m)=tSPC(1286)+iC4H7(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2593 (C7H10O3(2223))
      deltaHrxn(T=298K) = -7.129001023627069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8110000e+00 -6.1568000e-02 -4.0301000e-02 /
CHEB / 3.5863000e+00 6.9033000e-02 4.4865000e-02 /
CHEB / 9.3950000e-01 5.0981000e-03 3.6423000e-03 /
CHEB / 2.2422000e-01 -1.2184000e-02 -7.7249000e-03 /
CHEB / 3.8275000e-02 -2.8935000e-03 -2.0903000e-03 /

tSPC(1286)+iC4H7(+m)=tSPC(1553)+C4H7OJ(79)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2593 (C7H10O3(2223))
      deltaHrxn(T=298K) = -31.506743180358235 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2842000e+01 -1.3932000e-01 -9.2088000e-02 /
CHEB / -1.4257000e-01 1.5059000e-01 9.8225000e-02 /
CHEB / -1.4955000e-02 2.3393000e-02 1.6316000e-02 /
CHEB / -1.7134000e-02 -2.9917000e-02 -1.8170000e-02 /
CHEB / -1.2401000e-02 -1.3981000e-02 -9.7897000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!Here are the path reactions and their high-P limit kinetics:
```

```
C3H3O-enone+tSPC(122)(+m)=tSPC(1286)+tSPC(77)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2923 (C7H10O5(2228))
      deltaHrxn(T=298K) = -7.129000984762527 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0073000e+00 -1.6552000e-01 -9.7079000e-02 /
CHEB / 2.9258000e+00 1.7070000e-01 9.6042000e-02 /
CHEB / 5.7855000e-01 1.9432000e-03 4.0913000e-03 /
CHEB / 4.5472000e-02 -2.0183000e-02 -1.0635000e-02 /
CHEB / -2.5307000e-02 4.9699000e-03 2.1946000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:

tSPC(122)+tSPC(346)(+m)=tSPC(77)+tSPC(878)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H10O5(418)) deltaHrxn(T=298K)
= -26.257465107404073 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9810000e+00 -6.6025000e-05 -4.5957000e-05 /
CHEB / 3.1782000e+00 6.2517000e-05 4.3515000e-05 /
CHEB / 9.4430000e-01 1.3810000e-05 9.6124000e-06 /
CHEB / 2.0997000e-01 -8.0675000e-06 -5.6152000e-06 /
CHEB / 1.3725000e-02 -3.6955000e-06 -2.5723000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3O-2          29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C2H4O            -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

OH+tSPC(346)(+m)=C2H3O-2+HCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3663 (C3H4O2(2845))    deltaHrxn(T=298K) =
3.1899661216565924 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0199000e+01 -8.5357000e-01 -1.8884000e-01 /
CHEB / 2.1298000e+00 8.7444000e-01 1.2012000e-01 /
CHEB / 9.8817000e-02 1.1409000e-01 1.0198000e-01 /
CHEB / -1.1370000e-01 -8.1897000e-02 5.3116000e-03 /
CHEB / -5.6111000e-02 -5.4839000e-02 -2.7696000e-02 /

OH+tSPC(346)(+m)=C2H4O+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3663 (C3H4O2(2845))    deltaHrxn(T=298K) = -
92.72020834367072 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1862000e+01 -1.0645000e+00 -1.6262000e-01 /
CHEB / 6.3971000e-01 9.4862000e-01 4.7671000e-02 /
CHEB / 3.8730000e-02 2.5829000e-01 1.0896000e-01 /
CHEB / -1.0422000e-01 -4.0986000e-02 4.5055000e-02 /
CHEB / -7.6202000e-02 -7.8005000e-02 -1.1281000e-02 /

C2H3O-2+HCO(+m)=C2H4O+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3663 (C3H4O2(2845))    deltaHrxn(T=298K) = -
95.91017446532732 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1977000e+01 -9.4464000e-01 -1.9243000e-01 /
CHEB / 5.3494000e-01 8.7429000e-01 9.7555000e-02 /
CHEB / 3.0586000e-02 2.0524000e-01 1.0671000e-01 /
CHEB / -6.3759000e-02 -5.0902000e-02 2.7841000e-02 /
CHEB / -3.9910000e-02 -7.0039000e-02 -1.8185000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+HOC[CH2][CH3]2(+m)=tSPC(346)+tSPC(97)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4247 (C7H12O4(1456))
      deltaHrxn(T=298K) = -7.04935413201661 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6918000e+00 -2.5162000e-05 -1.7515000e-05 /
CHEB / 4.4927000e+00 2.1740000e-05 1.5133000e-05 /
CHEB / 1.1748000e+00 7.1916000e-06 5.0058000e-06 /
CHEB / 2.5723000e-01 -2.5827000e-06 -1.7977000e-06 /
CHEB / 2.1074000e-02 -1.7595000e-06 -1.2247000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+tSPC(97)(+m)=tSPC(1286)+HOC[CH2][CH3]2(+m)      1.0E0 0.0
0.0   !NetReaction from PDepNetwork #4597 (C7H12O4(2229))
      deltaHrxn(T=298K) = 7.109589468829238 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0002000e+00 -7.8466000e-02 -5.0322000e-02 /
CHEB / 6.1367000e+00 9.1292000e-02 5.7875000e-02 /
CHEB / 9.0340000e-01 1.0817000e-03 1.5138000e-03 /
CHEB / 1.2065000e-01 -1.4329000e-02 -8.9878000e-03 /
CHEB / -5.6474000e-02 -2.3989000e-03 -1.8839000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+CH3(+m)=tSPC(346)+sSPC(1697)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4963 (C4H6O3(1451))
      deltaHrxn(T=298K) = -5.059114761387502 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8151000e+00 -6.8341000e-06 -4.7570000e-06 /
CHEB / 3.0675000e+00 -5.7624000e-06 -4.0110000e-06 /
CHEB / 1.0128000e+00 -4.1700000e-06 -2.9026000e-06 /
CHEB / 3.1477000e-01 -4.2685000e-06 -2.9712000e-06 /
CHEB / 8.5792000e-02 -3.4318000e-06 -2.3888000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     CH3O             4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+sSPC(1697)(+m)=tSPC(1553)+CH3O(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #5257 (C4H6O3(2224))
      deltaHrxn(T=298K) = -38.42573009179217 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2695000e+01 3.1502000e-08 2.1721000e-08 /
CHEB / 1.0340000e-01 1.0776000e-07 7.4876000e-08 /
CHEB / 9.8670000e-03 1.0392000e-07 7.2595000e-08 /
CHEB / 2.5100000e-02 7.0142000e-08 4.9091000e-08 /
CHEB / 9.3224000e-03 4.3462000e-08 3.0269000e-08 /

C3H3O-enone+sSPC(1697)(+m)=tSPC(1286)+CH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #5257 (C4H6O3(2224))
      deltaHrxn(T=298K) = 5.119350098200133 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4635000e+00 -2.4909000e-04 -1.7335000e-04 /
CHEB / 4.8339000e+00 1.6351000e-04 1.1379000e-04 /
CHEB / 9.0915000e-01 1.0828000e-04 7.5352000e-05 /
CHEB / 2.3074000e-01 -2.0816000e-06 -1.4448000e-06 /
CHEB / 7.5637000e-02 -2.0756000e-05 -1.4441000e-05 /

tSPC(1286)+CH3(+m)=tSPC(1553)+CH3O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5257 (C4H6O3(2224))     deltaHrxn(T=298K) = -
43.545080189992305 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3649000e+01 7.0615000e-08 4.9131000e-08 /
CHEB / -4.1473000e-01 1.6879000e-07 1.1748000e-07 /
CHEB / 8.8550000e-03 1.5564000e-07 1.0836000e-07 /
CHEB / 4.7570000e-02 1.1597000e-07 8.0746000e-08 /
CHEB / 2.2979000e-02 8.0085000e-08 5.5749000e-08 /

!PDepNetwork tSPC(1416)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!     HO2              3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(1553)  -19.27      73.08 18.28 22.22 25.51 28.12 31.86 34.37
      37.97  !MRH CBS-QB3 w/1DHR corrections
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(1286)  -11.0 79.85 22.68 26.88 30.42 33.26 37.32 39.96 43.51
!MRH CBS-QB3 w/1DHR corrections
!Here are the path reactions and their high-P limit kinetics:
!     OCOOH+C2H3=tSPC(1416)   1.4157154e+13      -0.15000
2.9166667e+02
!     C3H3O-enone+HO2=tSPC(1416)    1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(1553)+OH=tSPC(1416)      2.0000000e+13      0.00000
0.0000000e+00
!     tSPC(1286)+H=tSPC(1416) 1.4157154e+13      -0.15000
2.9166667e+02

OCOOH+C2H3(+m)=tSPC(1416)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/NonDe     Cd_pri_rad          deltaHrxn(T=298K) = -
108.4986925398034 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6935000e+00 1.9886000e+00 -7.8741000e-03 /
CHEB / -9.2871000e-01 8.7129000e-03 6.0110000e-03 /
CHEB / -3.6036000e-01 3.5780000e-03 2.4694000e-03 /
CHEB / -3.8130000e-02 -8.0826000e-04 -5.5091000e-04 /
CHEB / 5.7444000e-02 -1.0993000e-03 -7.5723000e-04 /

C3H3O-enone+HO2(+m)=tSPC(1416)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/OneDe     O_rad/NonDe         deltaHrxn(T=298K) = -
88.62108415119619 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9980000e+00 1.9353000e+00 -4.2907000e-02 /
CHEB / -9.1712000e-01 5.4985000e-02 3.6158000e-02 /
CHEB / -4.9458000e-01 1.7922000e-02 1.1880000e-02 /
CHEB / -1.3701000e-01 -5.3225000e-03 -3.2679000e-03 /
CHEB / 1.1938000e-03 -5.5697000e-03 -3.6472000e-03 /

OCOOH+C2H3(+m)=C3H3O-enone+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416))   deltaHrxn(T=298K) = -19.877608388607218
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

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CHEB / 5    3 /
CHEB / 9.6672000e+00 -9.3985000e-03 -6.4973000e-03 /
CHEB / 7.5387000e-01 8.7728000e-03 6.0577000e-03 /
CHEB / 4.4377000e-01 2.0793000e-03 1.4401000e-03 /
CHEB / 1.7339000e-01 -1.2012000e-03 -8.2483000e-04 /
CHEB / 5.1797000e-02 -7.8539000e-04 -5.4372000e-04 /

tSPC(1553)+OH(+m)=tSPC(1416)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     O_pri_rad      deltaHrxn(T=298K) = -
50.454750235893655 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2767000e+01 5.2393000e-01 -5.9932000e-02 /
CHEB / -1.2287000e+00 8.2797000e-01 -5.6937000e-02 /
CHEB / -7.3829000e-01 4.3247000e-01 1.8297000e-02 /
CHEB / -3.6112000e-01 1.3599000e-01 3.6534000e-02 /
CHEB / -1.3642000e-01 9.5856000e-04 1.9276000e-02 /

OCOOH+C2H3(+m)=tSPC(1553)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416))   deltaHrxn(T=298K) = -58.043942303909745
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3022000e+01 -1.0762000e-02 -7.4362000e-03 /
CHEB / -2.6732000e-01 8.9248000e-03 6.1591000e-03 /
CHEB / -8.3931000e-03 3.1851000e-03 2.2003000e-03 /
CHEB / 3.5640000e-02 -9.8260000e-04 -6.7171000e-04 /
CHEB / 1.8854000e-02 -1.0366000e-03 -7.1502000e-04 /

C3H3O-enone+HO2(+m)=tSPC(1553)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(1416))    deltaHrxn(T=298K) = -
38.16633391530253 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2626000e+01 -5.9034000e-02 -3.9183000e-02 /
CHEB / -1.7841000e-03 5.5532000e-02 3.6610000e-02 /
CHEB / -2.9781000e-02 1.3457000e-02 9.0205000e-03 /
CHEB / -1.8764000e-02 -6.9631000e-03 -4.3981000e-03 /
CHEB / -1.9428000e-02 -4.9485000e-03 -3.2984000e-03 /

tSPC(1286)+H(+m)=tSPC(1416)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
102.12916712751988 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6635000e+00 1.9793000e+00 -1.4190000e-02 /
CHEB / -8.4090000e-01 1.6531000e-02 1.1317000e-02 /
CHEB / -4.1138000e-01 6.2624000e-03 4.2921000e-03 /
CHEB / -9.2680000e-02 -1.6114000e-03 -1.0801000e-03 /
CHEB / 2.7262000e-02 -1.9324000e-03 -1.3197000e-03 /

tSPC(1286)+H(+m)=OCOOH+C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416))   deltaHrxn(T=298K) = 6.369525412283522
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

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CHEB / 5    3 /
CHEB / 5.8805000e+00 -8.2295000e-03 -5.6929000e-03 /
CHEB / 4.6837000e+00 8.0833000e-03 5.5852000e-03 /
CHEB / 7.3960000e-01 1.3407000e-03 9.3150000e-04 /
CHEB / 1.9171000e-01 -1.0800000e-03 -7.4341000e-04 /
CHEB / 3.9008000e-02 -5.7531000e-04 -3.9930000e-04 /

tSPC(1286)+H(+m)=C3H3O-enone+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(1416))    deltaHrxn(T=298K) = -
13.508082976323688 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8853000e+00 -1.5833000e-02 -1.0885000e-02 /
CHEB / 1.2985000e+00 1.5811000e-02 1.0848000e-02 /
CHEB / 5.0412000e-01 2.5624000e-03 1.7758000e-03 /
CHEB / 1.3568000e-01 -2.2177000e-03 -1.5102000e-03 /
CHEB / 2.4135000e-02 -1.1038000e-03 -7.6412000e-04 /

tSPC(1286)+H(+m)=tSPC(1553)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(1416))   deltaHrxn(T=298K) = -51.67441689162621
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2762000e+01 -1.9318000e-02 -1.3262000e-02 /
CHEB / -9.9338000e-02 1.6847000e-02 1.1540000e-02 /
CHEB / -2.2702000e-02 5.3134000e-03 3.6492000e-03 /
CHEB / -4.1050000e-03 -1.9975000e-03 -1.3473000e-03 /
CHEB / -5.3458000e-03 -1.7899000e-03 -1.2265000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     pC3H3             81.58 59.57 13.76 16.14 18.14 19.8  22.39 24.34
      27.47 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!Here are the path reactions and their high-P limit kinetics:

HO2+pC3H3(+m)=tSPC(346)+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9052 (C3H4O2JJ(1771))  deltaHrxn(T=298K) = -
45.30579563371905 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0142000e+01 -2.0725000e-13 -1.4585000e-13 /
CHEB / 2.4786000e+00 -3.6636000e-13 -2.5212000e-13 /
CHEB / -4.1705000e-01 -2.2406000e-13 -1.5860000e-13 /
CHEB / -9.0194000e-03 -4.7865000e-14 -3.0987000e-14 /
CHEB / 2.6537000e-02 1.1691000e-13 7.9769000e-14 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+tSPC(1286)(+m)=tSPC(1553)+tSPC(1553)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #33 (C6H6O4JJ(395))
      deltaHrxn(T=298K) = -51.20447590612865 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3653000e+01 -2.9822000e-04 -2.5240000e-04 /
CHEB / -7.6464000e-01 2.4905000e-05 2.0549000e-05 /
CHEB / 1.2712000e-03 4.1162000e-04 3.4818000e-04 /
CHEB / 2.9065000e-02 5.1590000e-05 4.3317000e-05 /
CHEB / 9.6446000e-03 -1.7918000e-04 -1.5173000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
tSPC(878)+C3H3O-enone(+m)=tSPC(1286)+tSPC(346)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #100 (C6H6O4(364))
      deltaHrxn(T=298K) = 0.060235336812635154 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9130000e+00 -1.8321000e-05 -1.2752000e-05 /
CHEB / 5.4701000e+00 5.5601000e-06 3.8702000e-06 /
CHEB / 1.2842000e+00 7.8882000e-06 5.4907000e-06 /
CHEB / 3.4112000e-01 1.8999000e-06 1.3225000e-06 /
CHEB / 6.9452000e-02 -2.5936000e-07 -1.8052000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H5O-1           -7.2  70.51 14.71 17.83 20.61 23.05 26.99 29.97
      32.69 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

C2H4O+HCO(+m)=C3H3O-enone+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (C3H5O2J(511))     deltaHrxn(T=298K) = -
28.007500416399026 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.1721000e+00 -4.3161000e-02 -3.2215000e-02 /
CHEB / 6.4594000e+00 5.4492000e-02 4.0662000e-02 /
CHEB / 3.5838000e-01 -3.7790000e-03 -2.9143000e-03 /
CHEB / 1.3112000e-01 -1.0214000e-02 -7.4098000e-03 /
CHEB / 5.2652000e-02 6.2279000e-04 3.9237000e-04 /

C3H4O+OH(+m)=C3H3O-enone+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (C3H5O2J(511))     deltaHrxn(T=298K) = -
36.21645015615513 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0382000e+00 -4.3161000e-02 -3.2215000e-02 /
CHEB / 3.8501000e+00 5.4492000e-02 4.0662000e-02 /
CHEB / 3.4866000e-01 -3.7790000e-03 -2.9143000e-03 /
```

```
CHEB / 1.2134000e-01 -1.0214000e-02 -7.4098000e-03 /
CHEB / 4.3915000e-02 6.2279000e-04 3.9237000e-04 /

C2H5O-1+CO(+m)=C3H3O-enone+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #237 (C3H5O2J(511))     deltaHrxn(T=298K) = -
13.598954911217817 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1365000e+01 -9.8330000e-05 -6.8465000e-05 /
CHEB / 2.7089000e+01 7.0750000e-05 4.9264000e-05 /
CHEB / 7.4227000e-01 3.5434000e-05 2.4673000e-05 /
CHEB / 2.8115000e-01 -3.0757000e-07 -2.1680000e-07 /
CHEB / 1.1271000e-01 -5.3809000e-06 -3.7479000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     CH2CO            -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+CH2CHO(+m)=CH2O+C3H3O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #315 (C4H5O2J(606))      deltaHrxn(T=298K) = -
10.319153441865735 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.6712000e+00 -2.5761000e-01 -1.3271000e-01 /
CHEB / 1.5041000e+01 3.4277000e-01 1.6941000e-01 /
CHEB / 4.2307000e-02 -5.7732000e-02 -1.7983000e-02 /
CHEB / -1.5183000e-01 -4.8172000e-02 -2.7381000e-02 /
CHEB / -2.5057000e-02 1.7215000e-02 5.3465000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO            -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+CH2CHO(+m)=CH2C[O]CH3+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #434 (C4H5O2J(752))     deltaHrxn(T=298K) = -
24.2777105270231 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3371000e+01 -4.2880000e-02 -2.8945000e-02 /
CHEB / 2.1443000e+01 3.9915000e-02 2.6731000e-02 /
CHEB / -7.3660000e-02 6.6951000e-03 4.6367000e-03 /
CHEB / -9.5072000e-02 -5.1736000e-03 -3.3869000e-03 /
CHEB / -7.5635000e-02 -1.8021000e-03 -1.2443000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!Here are the path reactions and their high-P limit kinetics:

tSPC(1416)+O(+m)=tSPC(1286)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H4O4JJ(370))      deltaHrxn(T=298K) = -
4.719524645103151 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0190000e+01 -8.6255000e-08 -6.0040000e-08 /
CHEB / 1.8263000e+00 -1.6906000e-07 -1.1768000e-07 /
CHEB / 3.6060000e-02 -1.5888000e-07 -1.1060000e-07 /
CHEB / 1.3010000e-02 -1.4250000e-07 -9.9190000e-08 /
CHEB / 7.9950000e-03 -1.2069000e-07 -8.4011000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(1416)+O(+m)=tSPC(1553)+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #779 (C3H4O4JJ(884))    deltaHrxn(T=298K) = -
25.797063940097644 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0671000e+01 -3.8234000e-07 -2.6614000e-07 /
CHEB / 1.4519000e+00 -7.4709000e-07 -5.2003000e-07 /
CHEB / 4.3929000e-02 -6.9597000e-07 -4.8445000e-07 /
CHEB / 2.5779000e-02 -6.1591000e-07 -4.2872000e-07 /
CHEB / 1.4774000e-02 -5.1333000e-07 -3.5732000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+C4H7OJ(79)(+m)=tSPC(1553)+iC4H7(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1064 (C7H10O2JJ(1182))
      deltaHrxn(T=298K) = -19.697732725770408 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1524000e+01 -2.1710000e-01 7.1370000e-02 /
CHEB / 1.2169000e+00 -3.9217000e-02 -5.7352000e-02 /
CHEB / 1.7643000e-01 1.3208000e-01 -5.6038000e-02 /
CHEB / -4.7959000e-02 1.9227000e-01 -2.3631000e-02 /
CHEB / -9.7129000e-02 6.7625000e-02 3.7846000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+CH2CHO(+m)=CH2CO+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1572 (C4H6O2(686))     deltaHrxn(T=298K) = -
53.52468692572742 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0092000e+01 -1.3787000e+00 -6.2723000e-02 /
CHEB / 1.7466000e+00 9.7312000e-01 -5.7016000e-02 /
CHEB / 3.2163000e-01 4.5464000e-01 3.7129000e-02 /
CHEB / -1.3339000e-01 7.3215000e-02 5.6617000e-02 /
CHEB / -1.0993000e-01 -7.0744000e-02 2.5064000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
```

```
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!Here are the path reactions and their high-P limit kinetics:

CH3O+C3H3O-enone(+m)=CH3+tSPC(1553)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1744 (C4H6O2(1391))     deltaHrxn(T=298K) = -
7.659395716136345 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0721000e+01 -1.0689000e+00 -1.6427000e-01 /
CHEB / 1.2544000e+00 9.4856000e-01 4.0260000e-02 /
CHEB / 3.2432000e-01 2.5209000e-01 1.1434000e-01 /
CHEB / -3.5221000e-02 -3.2895000e-02 4.6266000e-02 /
CHEB / -5.4342000e-02 -7.7035000e-02 -1.1049000e-02 /

CH3+tSPC(1553)(+m)=C3H6+CO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1744 (C4H6O2(1391))    deltaHrxn(T=298K) = -
96.4798326450818 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1833000e+01 -1.2955000e+00 -1.0807000e-01 /
CHEB / 7.8024000e-01 9.7478000e-01 -4.5126000e-02 /
CHEB / 2.0297000e-01 3.9806000e-01 7.7070000e-02 /
CHEB / -4.8319000e-02 4.3371000e-02 7.4661000e-02 /
CHEB / -5.9188000e-02 -7.2071000e-02 2.1459000e-02 /

CH3O+C3H3O-enone(+m)=C3H6+CO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1744 (C4H6O2(1391))    deltaHrxn(T=298K) = -
104.13922836121816 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2247000e+01 -1.1620000e+00 -1.5400000e-01 /
CHEB / 3.2884000e-01 9.3597000e-01 9.9106000e-03 /
CHEB / 1.2129000e-01 3.2260000e-01 9.9909000e-02 /
CHEB / -6.5958000e-02 9.3888000e-03 6.2798000e-02 /
CHEB / -6.7474000e-02 -6.9488000e-02 4.7277000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
```

```
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+CH2CHO(+m)=C3H6+CO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1924 (C4H6O2(759))     deltaHrxn(T=298K) = -
93.40041166136788 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2413000e+01 -6.1710000e-01 -2.0327000e-01 /
CHEB / -1.1307000e-01 6.6906000e-01 1.8343000e-01 /
CHEB / -1.6826000e-01 4.9032000e-02 5.7394000e-02 /
CHEB / -1.2740000e-01 -8.0920000e-02 -1.6821000e-02 /
CHEB / -3.8362000e-02 -3.2682000e-02 -2.1933000e-02 /

CH3CO+CH2CHO(+m)=CH2CO+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1924 (C4H6O2(759))     deltaHrxn(T=298K) = -
44.95551677278859 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5367000e+00 -5.3196000e-01 -1.8848000e-01 /
CHEB / 1.8352000e+00 6.1883000e-01 1.8804000e-01 /
CHEB / 3.0454000e-01 -9.9502000e-03 3.9130000e-02 /
CHEB / 3.3963000e-02 -6.8161000e-02 -2.5705000e-02 /
CHEB / 3.8355000e-02 -2.2447000e-02 -1.8491000e-02 /

CH2CO+C2H4O(+m)=C3H6+CO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1924 (C4H6O2(759))     deltaHrxn(T=298K) = -
48.444894888579284 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2308000e+00 -8.1205000e-01 -1.8597000e-01 /
CHEB / 1.5147000e+01 8.5185000e-01 1.3123000e-01 /
CHEB / 2.0281000e-01 9.0559000e-02 8.8223000e-02 /
CHEB / -3.1880000e-02 -9.2931000e-02 -1.4054000e-03 /
CHEB / -4.9217000e-03 -4.8366000e-02 -2.7915000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+sC3H5(+m)=HCO+CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2112 (C4H6O2(2512))     deltaHrxn(T=298K) = -
15.758674996340257 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2786000e+01 -4.2357000e-01 -1.8645000e-01 /
CHEB / -2.5633000e-01 4.6051000e-01 1.8441000e-01 /
CHEB / 6.5621000e-02 3.3009000e-02 3.3770000e-02 /
CHEB / -2.7578000e-02 -6.1213000e-02 -2.0837000e-02 /
CHEB / -9.4781000e-03 -2.1942000e-02 -1.5982000e-02 /

HCO+CH2C[O]CH3(+m)=CO+H2CCCH3[OH](+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2112 (C4H6O2(2512))     deltaHrxn(T=298K) = -
72.71265611499598 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1093000e+01 -9.2042000e-01 -1.9151000e-01 /
CHEB / 7.7151000e-01 8.8317000e-01 9.8788000e-02 /
CHEB / 1.9877000e-01 1.6702000e-01 1.0601000e-01 /
CHEB / -2.9574000e-02 -7.2425000e-02 2.0497000e-02 /
CHEB / -1.8405000e-02 -6.4920000e-02 -2.3698000e-02 /

sSPC(2810)+sC3H5(+m)=CO+H2CCCH3[OH](+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2112 (C4H6O2(2512))     deltaHrxn(T=298K) = -
88.47133111133624 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1222000e+01 -4.5907000e-01 -1.9940000e-01 /
CHEB / 4.9983000e-01 4.6780000e-01 1.8295000e-01 /
CHEB / 1.4861000e-01 6.7029000e-02 4.6404000e-02 /
CHEB / 1.9696000e-02 -5.8820000e-02 -1.5742000e-02 /
CHEB / 9.4174000e-03 -2.9966000e-02 -1.7589000e-02 /

HCO+CH2C[O]CH3(+m)=CO2+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2112 (C4H6O2(2512))    deltaHrxn(T=298K) = -
96.87984031759217 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2647000e+01 -9.2913000e-01 -1.9211000e-01 /
CHEB / -9.7846000e-02 8.8167000e-01 9.6232000e-02 /
CHEB / -4.2669000e-02 1.7525000e-01 1.0601000e-01 /
CHEB / -1.1091000e-01 -6.8883000e-02 2.2925000e-02 /
CHEB / -5.1629000e-02 -6.5428000e-02 -2.2299000e-02 /
```

```
sSPC(2810)+sC3H5(+m)=CO2+C3H6(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2112 (C4H6O2(2512))    deltaHrxn(T=298K) = -
112.63851531393243 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2680000e+01 -4.6218000e-01 -2.0061000e-01 /
CHEB / -3.0310000e-01 4.6771000e-01 1.8253000e-01 /
CHEB / -8.0741000e-02 7.0086000e-02 4.7505000e-02 /
CHEB / -6.1584000e-02 -5.8025000e-02 -1.5067000e-02 /
CHEB / -2.2974000e-02 -3.0553000e-02 -1.7601000e-02 /

CO+H2CCCH3[OH](+m)=CO2+C3H6(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2112 (C4H6O2(2512))    deltaHrxn(T=298K) = -
24.167184202596186 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4045000e+01 -1.3117000e+00 -8.0437000e-02 /
CHEB / 2.1501000e+01 1.0270000e+00 -5.8200000e-02 /
CHEB / 4.6135000e-01 4.0395000e-01 6.6719000e-02 /
CHEB / -4.8514000e-02 5.1585000e-03 7.4512000e-02 /
CHEB / -2.8909000e-02 -9.6542000e-02 2.0300000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C3H6O             -44.5 72.73 19.42 23.41 26.92 29.97 35.32 39.17
      43.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     acetone     -51.56      70.09 17.97 22.0  25.89 29.34 34.93 39.15
      44.77 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+HCO(+m)=CH3CO+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) = -
3.4794286562242904 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1027000e+01 -1.2059000e+00 -8.4686000e-02 /
CHEB / 1.4822000e+00 1.0479000e+00 -1.2954000e-02 /
CHEB / 1.0204000e-01 3.2459000e-01 8.1508000e-02 /
```

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CHEB / -1.4366000e-01 -3.1368000e-02 4.6286000e-02 /
CHEB / -8.5189000e-02 -9.1534000e-02 -3.1585000e-03 /

CH3CO+CH2CHO(+m)=C3H6O+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) = -
74.9227434373625 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1981000e+00 -3.0457000e-01 -1.5604000e-01 /
CHEB / 1.1133000e+01 2.9154000e-01 1.4473000e-01 /
CHEB / 3.8584000e-01 7.1875000e-02 3.8810000e-02 /
CHEB / 9.9438000e-02 -3.3407000e-02 -1.2075000e-02 /
CHEB / 1.9828000e-02 -2.5531000e-02 -1.3190000e-02 /

CH2C[O]CH3+HCO(+m)=C3H6O+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) = -
78.40217209358678 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6039000e-01 -2.9684000e-01 -1.5264000e-01 /
CHEB / 1.0091000e+01 2.9052000e-01 1.4467000e-01 /
CHEB / 4.8602000e-01 6.4267000e-02 3.5528000e-02 /
CHEB / 1.4751000e-01 -3.5454000e-02 -1.3440000e-02 /
CHEB / 4.1600000e-02 -2.4096000e-02 -1.2849000e-02 /

CH3CO+CH2CHO(+m)=acetone+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) = -
81.9817899222851 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9842000e+00 -1.2059000e+00 -8.4686000e-02 /
CHEB / 3.8170000e+00 1.0479000e+00 -1.2954000e-02 /
CHEB / 3.7255000e-01 3.2459000e-01 8.1508000e-02 /
CHEB / -6.3892000e-02 -3.1368000e-02 4.6286000e-02 /
CHEB / -5.8190000e-02 -9.1534000e-02 -3.1585000e-03 /

CH2C[O]CH3+HCO(+m)=acetone+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) = -
85.4612185785094 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4620000e+00 -1.1409000e+00 -1.0120000e-01 /
CHEB / 3.2153000e+00 1.0380000e+00 6.4165000e-03 /
CHEB / 4.3969000e-01 2.7228000e-01 9.1223000e-02 /
CHEB / -1.3768000e-02 -5.2012000e-02 3.8536000e-02 /
CHEB / -2.9617000e-02 -8.7802000e-02 -9.6725000e-03 /

acetone+CO(+m)=C3H6O+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C4H6O2(2686))    deltaHrxn(T=298K) =
7.059046484922604 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6212000e+01 -2.9684000e-01 -1.5264000e-01 /
CHEB / 4.0421000e+01 2.9052000e-01 1.4467000e-01 /
CHEB / 8.0846000e-01 6.4267000e-02 3.5528000e-02 /
CHEB / 2.5316000e-01 -3.5454000e-02 -1.3440000e-02 /
CHEB / 8.4023000e-02 -2.4096000e-02 -1.2849000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+O(+m)=sSPC(2810)+sC3H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #126 (C4H6O2JJ(3614))    deltaHrxn(T=298K) = -
8.958666455345579 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1003000e+01 -1.3166000e-04 -9.2099000e-05 /
CHEB / 1.1820000e+00 1.8535000e-04 1.2972000e-04 /
CHEB / 4.4209000e-02 -4.3937000e-05 -3.0859000e-05 /
CHEB / 2.4358000e-02 -2.5356000e-05 -1.7666000e-05 /
CHEB / 1.3998000e-02 1.6363000e-05 1.1459000e-05 /

O+tSPC(110)(+m)=sSPC(2810)+sC3H5(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #126 (C4H6O2JJ(3614))    deltaHrxn(T=298K) = -
62.36326573332626 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3054000e+01 -3.5139000e-10 -2.4460000e-10 /
CHEB / -5.6338000e-02 4.8623000e-11 3.3850000e-11 /
CHEB / -1.0886000e-02 2.7066000e-10 1.8840000e-10 /
CHEB / -3.9450000e-03 1.3519000e-10 9.4106000e-11 /
CHEB / -6.9792000e-03 1.9011000e-11 1.3230000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+O(+m)=CH2C[O]CH3+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #183 (C4H6O2JJ(2730))   deltaHrxn(T=298K) = -
24.717341451685833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0571000e+01 -1.3153000e-05 -9.1554000e-06 /
CHEB / 1.4399000e+00 -2.2591000e-05 -1.5725000e-05 /
CHEB / -1.3876000e-02 -1.8091000e-05 -1.2593000e-05 /
CHEB / -1.0433000e-02 -1.3318000e-05 -9.2696000e-06 /
CHEB / -1.6429000e-02 -8.7297000e-06 -6.0763000e-06 /

tSPC(110)+O(+m)=CH2C[O]CH3+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #183 (C4H6O2JJ(2730))   deltaHrxn(T=298K) = -
78.12194072966652 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3996000e+01 -9.5651000e-06 -6.6579000e-06 /
CHEB / -9.7951000e-01 -1.6846000e-05 -1.1726000e-05 /
CHEB / -8.3157000e-02 -1.3586000e-05 -9.4565000e-06 /
CHEB / -5.0183000e-02 -1.0013000e-05 -6.9699000e-06 /
CHEB / -4.1336000e-02 -6.5949000e-06 -4.5904000e-06 /

tSPC(110)+O(+m)=C4H6Oi-13+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #183 (C4H6O2JJ(2730))   deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2361000e+00 -9.0451000e-06 -6.2960000e-06 /
CHEB / 8.0347000e-01 -1.5861000e-05 -1.1040000e-05 /
CHEB / 5.0234000e-01 -1.2737000e-05 -8.8654000e-06 /
CHEB / 1.6560000e-01 -9.3402000e-06 -6.5013000e-06 /
CHEB / 3.6115000e-02 -6.1035000e-06 -4.2483000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO            -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+HCO(+m)=CH2CHO+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #294 (C3H3O2J(385))     deltaHrxn(T=298K) = -
19.187969030308558 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0874000e+01 -3.0444000e-04 -2.1187000e-04 /
CHEB / 1.9277000e+01 -2.5462000e-05 -1.7703000e-05 /
CHEB / 2.4438000e-01 -1.2025000e-05 -8.3558000e-06 /
CHEB / 8.1749000e-02 -5.6998000e-05 -3.9654000e-05 /
CHEB / 1.9939000e-02 -4.3555000e-05 -3.0301000e-05 /

O+tSPC(346)(+m)=CH2CO+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #294 (C3H3O2J(385))     deltaHrxn(T=298K) = -
87.86095418067816 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3178000e+01 -7.9196000e-05 -5.5124000e-05 /
CHEB / -5.1195000e-01 -1.5292000e-05 -1.0642000e-05 /
CHEB / -1.6147000e-01 -4.6843000e-06 -3.2588000e-06 /
CHEB / -9.2150000e-02 -1.3872000e-05 -9.6540000e-06 /
CHEB / -5.4714000e-02 -1.0673000e-05 -7.4277000e-06 /

O+tSPC(346)(+m)=CH2CHO+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #294 (C3H3O2J(385))     deltaHrxn(T=298K) = -
107.04892321098671 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9877000e+00 -6.5891000e-05 -4.5863000e-05 /
CHEB / 1.4269000e+00 4.8456000e-06 3.3734000e-06 /
CHEB / 5.0117000e-01 7.4955000e-06 5.2176000e-06 /
CHEB / 1.5882000e-01 -6.2490000e-06 -4.3491000e-06 /
CHEB / 4.5398000e-02 -5.9679000e-06 -4.1536000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1553)  -19.27      73.08 18.28 22.22 25.51 28.12 31.86 34.37
      37.97  !MRH CBS-QB3 w/1DHR corrections
!     CO2              -94.36      50.99 8.87  9.84  10.63 11.26 12.23
      12.9  13.82
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
```

```
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H2CCCO      33.02 66.05 15.09 17.26 19.13 20.72 23.23 25.1  27.95
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!Here are the path reactions and their high-P limit kinetics:
!     CO2+C2H3=tSPC(1553)     3.2847733e+07      1.50370
7.3354000e+03
!     O+C3H3O-enone=tSPC(1553)      1.0000000e+13      0.00000
0.0000000e+00

tSPC(1553)(+m)=CO2+C2H3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553))   deltaHrxn(T=298K) = -2.8898814421128094
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9234000e+00 1.9998000e+00 -1.3498000e-04 /
CHEB / 7.0062000e-01 1.0464000e-04 7.2829000e-05 /
CHEB / -1.5774000e+00 2.2192000e-05 1.5445000e-05 /
CHEB / -6.6343000e-01 2.8899000e-06 2.0102000e-06 /
CHEB / -2.7324000e-01 -2.9545000e-07 -2.0612000e-07 /

OH+H2CCCO(+m)=tSPC(1553)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553))   deltaHrxn(T=298K) = -60.97325047651544
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3080000e+01 5.1296000e+00 -8.1890000e-01 /
CHEB / -7.8984000e-01 1.2561000e+00 8.7183000e-01 /
CHEB / -1.3583000e+00 2.0741000e-01 4.5167000e-01 /
CHEB / -6.5873000e-01 -8.4404000e-02 1.5105000e-01 /
CHEB / -3.3210000e-01 -1.1228000e-01 3.2177000e-02 /

OH+H2CCCO(+m)=CO2+C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553))   deltaHrxn(T=298K) = -63.86313191862824
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1531000e+00 -2.7971000e-01 -1.6508000e-01 /
CHEB / 2.1760000e+00 3.1814000e-01 1.7689000e-01 /
CHEB / 8.2871000e-02 1.0310000e-02 1.9462000e-02 /
CHEB / 2.2391000e-02 -4.1083000e-02 -2.1950000e-02 /
CHEB / 1.2866000e-02 -1.5178000e-02 -1.2637000e-02 /

O+C3H3O-enone(+m)=tSPC(1553)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553)) High-P Limit: Oa_R_Recombination estimate:
(Average:) Oa     CO_rad/OneDe      deltaHrxn(T=298K) = -
103.41921494757551 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1347000e+01 5.3593000e+00 1.7553000e+00 /
CHEB / -3.3609000e+00 2.5337000e-01 2.5079000e-01 /
CHEB / -1.5987000e+00 -2.2464000e-01 -3.5979000e-02 /
CHEB / -7.0899000e-01 -1.6731000e-01 -5.0913000e-02 /
```

```
CHEB / -3.2917000e-01 -1.1955000e-01 -4.0313000e-02 /

O+C3H3O-enone(+m)=CO2+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553))   deltaHrxn(T=298K) = -106.30909638968832
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3854000e+01 -3.0659000e-09 -2.1341000e-09 /
CHEB / -6.9237000e-01 4.6208000e-09 3.2166000e-09 /
CHEB / -1.2552000e-03 1.6517000e-09 1.1496000e-09 /
CHEB / 1.1817000e-02 1.9700000e-11 1.3547000e-11 /
CHEB / 3.2623000e-03 -4.2846000e-10 -2.9826000e-10 /

O+C3H3O-enone(+m)=OH+H2CCCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (tSPC(1553))   deltaHrxn(T=298K) = -42.44596447106009
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9364000e+00 -1.5879000e-02 -1.1217000e-02 /
CHEB / 4.7822000e-01 1.9222000e-02 1.3606000e-02 /
CHEB / 4.4888000e-01 -1.4970000e-03 -1.0955000e-03 /
CHEB / 1.6904000e-01 -2.0169000e-03 -1.4231000e-03 /
CHEB / 6.1438000e-02 -7.0508000e-05 -4.1054000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!Here are the path reactions and their high-P limit kinetics:

CO+CH2CHO(+m)=CO2+C2H3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #639 (C3H3O2J(1537))    deltaHrxn(T=298K) = -
2.2995466936455244 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5449000e+00 -1.3422000e-09 -9.3426000e-10 /
CHEB / 3.3651000e+00 -2.2353000e-09 -1.5560000e-09 /
CHEB / -5.2902000e-01 -1.0937000e-09 -7.6132000e-10 /
CHEB / -9.7224000e-02 2.4429000e-10 1.7005000e-10 /
CHEB / 5.0670000e-03 1.2661000e-09 8.8127000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+HCO(+m)=CH3CO+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #736 (C3H3O2J(750))     deltaHrxn(T=298K) = -
27.75713918324739 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2984000e+00 -4.6597000e-04 -3.2427000e-04 /
CHEB / 1.6067000e+01 2.3245000e-04 1.6175000e-04 /
CHEB / 2.9963000e-01 1.2506000e-04 8.7021000e-05 /
CHEB / 9.8322000e-02 -1.8773000e-05 -1.3057000e-05 /
CHEB / 1.1362000e-02 -4.3231000e-05 -3.0080000e-05 /

CH2CHO+CO(+m)=CH3CO+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #736 (C3H3O2J(750))     deltaHrxn(T=298K) = -
8.569170152938831 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4211000e+01 -4.7652000e-04 -3.3161000e-04 /
CHEB / 2.2297000e+01 2.2096000e-04 1.5375000e-04 /
CHEB / 1.2705000e-01 1.2292000e-04 8.5533000e-05 /
CHEB / 2.4108000e-02 -1.9775000e-05 -1.3754000e-05 /
CHEB / -1.5863000e-02 -4.5566000e-05 -3.1704000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
C2H3+tSPC(1553)(+m)=CH2CHO+C3H3O-enone(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1062 (C5H6O2(688))
      deltaHrxn(T=298K) = -27.027505221026033 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3851000e+01 -1.6519000e-01 -1.0475000e-01 /
CHEB / -8.9295000e-01 1.9213000e-01 1.1922000e-01 /
CHEB / 1.6540000e-02 4.5973000e-03 5.7498000e-03 /
CHEB / 8.9302000e-03 -3.2189000e-02 -1.8930000e-02 /
CHEB / 1.5631000e-02 -5.8466000e-03 -5.1661000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H5OJ(15) 8.76  72.88 22.52 27.78 31.88 35.05 39.89 43.1  46.9
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(346)+CH2CHO(+m)=iC4H5OJ(15)+HCO(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1995 (C5H6O2JJ(639))    deltaHrxn(T=298K) = -
14.508737718496441 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7398000e+00 -1.3928000e-03 -9.6918000e-04 /
CHEB / 2.9346000e+00 1.7900000e-03 1.2455000e-03 /
CHEB / 3.8482000e-02 -2.7518000e-04 -1.9136000e-04 /
CHEB / -4.0144000e-02 -1.5660000e-04 -1.0897000e-04 /
CHEB / -3.8497000e-02 2.1106000e-05 1.4608000e-05 /

tSPC(346)+CH2CHO(+m)=tSPC(110)+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1995 (C5H6O2JJ(639))    deltaHrxn(T=298K) = -
34.01672397803475 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1481000e+01 -3.1167000e-05 -2.1695000e-05 /
CHEB / 1.8575000e+01 2.4663000e-05 1.7168000e-05 /
CHEB / 4.5641000e-01 1.0687000e-05 7.4393000e-06 /
CHEB / 1.4408000e-01 -1.5386000e-06 -1.0711000e-06 /
CHEB / 3.0929000e-02 -2.1386000e-06 -1.4887000e-06 /
```

```
iC4H5OJ(15)+HCO(+m)=tSPC(110)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1995 (C5H6O2JJ(639))    deltaHrxn(T=298K) = -
19.507986259538303 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5246000e+01 -8.3709000e-07 -5.8280000e-07 /
CHEB / 2.2940000e+01 2.8670000e-07 1.9962000e-07 /
CHEB / 2.4665000e-01 7.5733000e-07 5.2725000e-07 /
CHEB / 1.0874000e-01 1.6111000e-07 1.1215000e-07 /
CHEB / 4.2946000e-02 -1.1337000e-07 -7.8942000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(346)+CH3CO(+m)=tSPC(110)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2766 (C5H6O2JJ(2644))   deltaHrxn(T=298K) = -
25.447553825095913 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2525000e+01 -3.3432000e-07 -2.3271000e-07 /
CHEB / 2.8220000e+01 3.6411000e-08 2.5345000e-08 /
CHEB / 4.4642000e-01 2.2313000e-07 1.5532000e-07 /
CHEB / 1.8085000e-01 1.0114000e-07 7.0402000e-08 /
CHEB / 7.6312000e-02 5.0380000e-09 3.5064000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

CH2OH+HCO(+m)=CH2CO+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3282 (C2H4O2(755))     deltaHrxn(T=298K) = -
75.94243192379479 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2020000e+01 -9.3628000e-01 -1.9192000e-01 /
CHEB / 3.8922000e-01 8.8706000e-01 9.5090000e-02 /
CHEB / -4.2124000e-02 1.8370000e-01 1.1258000e-01 /
CHEB / -4.7259000e-02 -5.5780000e-02 2.7710000e-02 /
CHEB / -2.6297000e-02 -6.3002000e-02 -2.0433000e-02 /

CH2CHO+OH(+m)=CH2CO+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3282 (C2H4O2(755))     deltaHrxn(T=298K) = -
84.7415011356084 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2105000e+01 -5.3430000e-01 -2.1670000e-01 /
CHEB / 1.5646000e-01 4.9470000e-01 1.8023000e-01 /
CHEB / -8.6679000e-02 1.3110000e-01 6.5487000e-02 /
CHEB / -6.0465000e-02 -4.2364000e-02 -2.2395000e-03 /
CHEB / -3.2749000e-02 -4.5526000e-02 -1.7725000e-02 /

CH2CO+H2O(+m)=CH3OH+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3282 (C2H4O2(755))     deltaHrxn(T=298K) = -
5.279191317980747 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0947000e+01 -7.5748000e-01 -2.1945000e-01 /
CHEB / 2.8339000e+01 7.1794000e-01 1.5689000e-01 /
CHEB / 1.2991000e-01 1.5990000e-01 8.6674000e-02 /
CHEB / 1.6324000e-02 -5.7484000e-02 1.1890000e-02 /
CHEB / -9.7307000e-03 -5.5538000e-02 -2.0103000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

HO2+C2H3(+m)=OH+CH2CHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3429 (C2H4O2(810))     deltaHrxn(T=298K) = -
56.43454815646077 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3115000e+01 1.0744000e-10 7.4787000e-11 /
CHEB / -3.9027000e-01 1.9570000e-10 1.3622000e-10 /
CHEB / -2.4297000e-02 1.5091000e-10 1.0504000e-10 /
CHEB / -4.7120000e-03 1.0017000e-10 6.9731000e-11 /
CHEB / -5.8658000e-03 5.7695000e-11 4.0158000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+C2H3(+m)=C4H7OJ(79)+CH2CHO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3761 (C6H10O2(1304))    deltaHrxn(T=298K) = -
65.66324942501134 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2907000e+01 4.6739000e-10 3.2534000e-10 /
CHEB / -2.1413000e-01 8.9618000e-10 6.2381000e-10 /
CHEB / -2.6756000e-02 7.9303000e-10 5.5201000e-10 /
CHEB / 1.7919000e-03 6.5178000e-10 4.5369000e-10 /
CHEB / -5.1745000e-03 4.9909000e-10 3.4740000e-10 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+sSPC(1590)(+m)=CH2C[O]CH3+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4054 (C6H10O2(2890))
      deltaHrxn(T=298K) = -34.667000066670674 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2740000e+01 -8.4155000e-01 -2.2489000e-01 /
CHEB / -3.4463000e-01 6.9111000e-01 1.3693000e-01 /
CHEB / -1.0113000e-02 2.4904000e-01 8.0526000e-02 /
CHEB / -1.6421000e-01 -2.8430000e-02 2.8728000e-02 /
CHEB / -1.3365000e-01 -6.3715000e-02 -1.0618000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     aC3H5            40.75 62.05 14.83 18.67 21.94 24.67 28.9  32.03
      36.9  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     HOC[CH2][CH3]2   -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
```

```
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!Here are the path reactions and their high-P limit kinetics:

HOC[CH2][CH3]2+C2H3(+m)=aC3H5+CH3C[OH]CH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4275 (C6H12O(1772))
      deltaHrxn(T=298K) = -27.86722500267283 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1212000e+01 -1.2273000e+00 -8.6281000e-02 /
CHEB / 6.8743000e-01 1.0738000e+00 -2.0027000e-02 /
CHEB / -4.5285000e-02 3.7785000e-01 9.0447000e-02 /
CHEB / -2.4929000e-01 -4.4813000e-02 6.9169000e-02 /
CHEB / -1.5543000e-01 -1.3675000e-01 -4.2291000e-04 /

aC3H5+CH3C[OH]CH3(+m)=iC4H8+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4275 (C6H12O(1772))     deltaHrxn(T=298K) = -
51.05473469597371 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3059000e+00 -1.4159000e+00 -3.5785000e-02 /
CHEB / 3.5738000e+00 9.9021000e-01 -3.9319000e-02 /
CHEB / 3.8126000e-01 5.6984000e-01 2.4347000e-02 /
CHEB / -3.4106000e-01 1.4785000e-01 5.8560000e-02 /
CHEB / -2.7822000e-01 -9.9348000e-02 3.8952000e-02 /

HOC[CH2][CH3]2+C2H3(+m)=iC4H8+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4275 (C6H12O(1772))     deltaHrxn(T=298K) = -
78.92195969864655 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7054000e+00 -1.2445000e+00 -8.4018000e-02 /
CHEB / 1.6267000e+00 1.0674000e+00 -2.3145000e-02 /
CHEB / 1.7005000e-01 3.9863000e-01 8.7114000e-02 /
CHEB / -1.6222000e-01 -2.7947000e-02 7.2743000e-02 /
CHEB / -1.1883000e-01 -1.3682000e-01 4.5797000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     aC3H5             40.75 62.05 14.83 18.67 21.94 24.67 28.9  32.03
      36.9  null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
```

```
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     C2H4O            -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(439)+C2H3(+m)=C4H8O2(62)+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4474 (C6H12O3(1989))    deltaHrxn(T=298K) = -
77.58205682980662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0346000e+00 -1.5772000e-01 -9.2719000e-02 /
CHEB / 2.4708000e+00 1.8735000e-01 1.0714000e-01 /
CHEB / 8.4786000e-01 -8.1263000e-03 -1.2498000e-03 /
CHEB / 2.5506000e-01 -3.1529000e-02 -1.8530000e-02 /
CHEB / 6.7947000e-02 -2.1351000e-03 -2.5203000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O             4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+C2H3(+m)=CH3O+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4683 (C3H6O2(1433))    deltaHrxn(T=298K) = -
65.45323531281821 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2852000e+01 2.3016000e-10 1.6021000e-10 /
CHEB / -1.6894000e-01 4.4518000e-10 3.0988000e-10 /
CHEB / -2.6773000e-02 4.0308000e-10 2.8057000e-10 /
CHEB / 1.7788000e-03 3.4201000e-10 2.3807000e-10 /
CHEB / -5.1841000e-03 2.7129000e-10 1.8883000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+HO2(+m)=CH2C[O]CH3+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C3H6O2(2879)) deltaHrxn(T=298K) = -55.564653607695426
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3160000e+01 1.8432000e-11 1.2828000e-11 /
CHEB / -4.5119000e-01 3.5190000e-11 2.4499000e-11 /
CHEB / -3.3091000e-02 3.0670000e-11 2.1345000e-11 /
CHEB / -2.3783000e-02 2.4468000e-11 1.7035000e-11 /
CHEB / -1.8407000e-02 1.7921000e-11 1.2471000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(1286)+C2H3(+m)=tSPC(1553)+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #4 (C5H6O3(1024))  deltaHrxn(T=298K) = -
78.23198112715468 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2828000e+01 -1.4480000e-04 -1.0076000e-04 /
CHEB / -1.5015000e-01 -2.3726000e-04 -1.6509000e-04 /
CHEB / -2.7353000e-02 -1.9198000e-04 -1.3358000e-04 /
CHEB / 1.2628000e-03 -1.5187000e-04 -1.0567000e-04 /
CHEB / -5.6170000e-03 -1.0880000e-04 -7.5695000e-05 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!Here are the path reactions and their high-P limit kinetics:

HCO+C4H6Oi-13(+m)=CO2+iC4H7(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #89 (C5H7O2J(1452))     deltaHrxn(T=298K) = -
44.80512202136153 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9026000e-01 -5.6457000e-07 -4.2093000e-07 /
CHEB / 9.2477000e+00 7.0806000e-07 5.2995000e-07 /
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CHEB / 3.6172000e-01 1.7468000e-07 1.1797000e-07 /
CHEB / 1.4011000e-01 -1.0256000e-07 -8.1604000e-08 /
CHEB / 6.0775000e-02 -5.2293000e-08 -3.2688000e-08 /

HCO+tSPC(110)(+m)=CO2+iC4H7(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #89 (C5H7O2J(1452))     deltaHrxn(T=298K) = -
98.20972129934222 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2626000e+00 -1.3689000e-04 -9.5282000e-05 /
CHEB / 5.6212000e-01 1.1009000e-04 7.6627000e-05 /
CHEB / 7.4119000e-01 4.3854000e-05 3.0525000e-05 /
CHEB / 2.3709000e-01 -7.5520000e-06 -5.2565000e-06 /
CHEB / 6.6252000e-02 -9.4690000e-06 -6.5910000e-06 /

CO+iC4H7OJ(15)(+m)=CO2+iC4H7(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #89 (C5H7O2J(1452))     deltaHrxn(T=298K) = -
25.497065243956243 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2028000e+01 -1.3689000e-04 -9.5282000e-05 /
CHEB / 2.6461000e+01 1.1009000e-04 7.6627000e-05 /
CHEB / 1.0475000e+00 4.3854000e-05 3.0525000e-05 /
CHEB / 3.5043000e-01 -7.5520000e-06 -5.2565000e-06 /
CHEB / 1.1341000e-01 -9.4690000e-06 -6.5910000e-06 /

HCO+C4H6Oi-13(+m)=CO+iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #89 (C5H7O2J(1452))      deltaHrxn(T=298K) = -
19.308056777405287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0362000e+01 -6.6453000e-09 -4.6311000e-09 /
CHEB / 1.8510000e+01 1.8267000e-07 1.2716000e-07 /
CHEB / 3.2561000e-01 1.4019000e-07 9.7588000e-08 /
CHEB / 1.2691000e-01 5.7351000e-08 3.9920000e-08 /
CHEB / 5.5436000e-02 1.4756000e-08 1.0269000e-08 /

HCO+tSPC(110)(+m)=CO+iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #89 (C5H7O2J(1452))      deltaHrxn(T=298K) = -
72.71265605538598 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8818000e+00 -2.0303000e-04 -1.4131000e-04 /
CHEB / 4.2579000e+00 1.8883000e-04 1.3142000e-04 /
CHEB / 1.1772000e+00 3.7298000e-05 2.5962000e-05 /
CHEB / 3.1744000e-01 -1.6379000e-05 -1.1397000e-05 /
CHEB / 8.7459000e-02 -9.4898000e-06 -6.6050000e-06 /

CO+C4H7OJ(79)(+m)=CO2+iC4H7(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #89 (C5H7O2J(1452))     deltaHrxn(T=298K) = -
49.024784640441965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7526000e+00 1.3378000e-12 9.3015000e-13 /
CHEB / 6.4809000e-01 2.6219000e-12 1.8275000e-12 /
CHEB / 2.9882000e-03 2.4740000e-12 1.7201000e-12 /
CHEB / 3.5897000e-03 2.2252000e-12 1.5508000e-12 /
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CHEB / 2.2913000e-03 1.8944000e-12 1.3171000e-12 /

HCO+tSPC(110)(+m)=CO+C4H7OJ(79)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #89 (C5H7O2J(1452))     deltaHrxn(T=298K) = -
49.18493665890025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8843000e+00 -1.6781000e-04 -1.1680000e-04 /
CHEB / 1.0785000e+01 1.3981000e-04 9.7308000e-05 /
CHEB / 8.7488000e-01 4.9512000e-05 3.4462000e-05 /
CHEB / 2.8397000e-01 -1.1459000e-05 -7.9748000e-06 /
CHEB / 7.8216000e-02 -1.1285000e-05 -7.8547000e-06 /

CO+C4H7OJ(79)(+m)=CO+iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #89 (C5H7O2J(1452))      deltaHrxn(T=298K) = -
23.52771939648573 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0040000e+01 -1.6781000e-04 -1.1680000e-04 /
CHEB / 2.8859000e+01 1.3981000e-04 9.7308000e-05 /
CHEB / 1.2574000e+00 4.9512000e-05 3.4462000e-05 /
CHEB / 4.1216000e-01 -1.1459000e-05 -7.9748000e-06 /
CHEB / 1.2554000e-01 -1.1285000e-05 -7.8547000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

HCO+tSPC(110)(+m)=HCO+C4H6Oi-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #256 (C5H7O2J(2248))    deltaHrxn(T=298K) = -
53.404599277980694 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2717000e+01 -5.1056000e-05 -3.5536000e-05 /
CHEB / -6.1342000e-02 -7.2115000e-05 -5.0192000e-05 /
```

```
CHEB / -2.8952000e-02 -6.0177000e-05 -4.1883000e-05 /
CHEB / 1.5801000e-03 -4.6143000e-05 -3.2115000e-05 /
CHEB / -3.0930000e-03 -3.0765000e-05 -2.1412000e-05 /

CO+C4H7OJ(79)(+m)=HCO+C4H6Oi-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #256 (C5H7O2J(2248))    deltaHrxn(T=298K) = -
4.219662619080442 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7690000e+01 -4.5857000e-05 -3.1917000e-05 /
CHEB / 2.5077000e+01 -6.6237000e-05 -4.6102000e-05 /
CHEB / 2.6092000e-01 -5.4847000e-05 -3.8174000e-05 /
CHEB / 9.4328000e-02 -4.1741000e-05 -2.9052000e-05 /
CHEB / 2.8559000e-02 -2.7682000e-05 -1.9266000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!Here are the path reactions and their high-P limit kinetics:

CO2+tSPC(346)(+m)=CO2+C3H3O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #352 (C4H3O3J(1440))     deltaHrxn(T=298K) = -
16.798238594152792 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0548000e+01 -7.4359000e-01 -2.2901000e-01 /
CHEB / 2.7125000e+01 7.5691000e-01 1.7187000e-01 /
CHEB / 9.6689000e-02 1.1938000e-01 1.0413000e-01 /
CHEB / -9.6515000e-02 -6.6643000e-02 1.1591000e-03 /
CHEB / -7.9727000e-02 -6.2929000e-02 -3.2641000e-02 /
```

```
sSPC(2810)+H2CCCO(+m)=CO2+tSPC(346)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #352 (C4H3O3J(1440))     deltaHrxn(T=298K) = -
68.82413482772355 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0427000e+00 -7.3791000e-01 -2.0647000e-01 /
CHEB / 4.1688000e+00 7.9045000e-01 1.6083000e-01 /
CHEB / 3.4725000e-01 7.2233000e-02 9.2384000e-02 /
CHEB / -3.0672000e-02 -8.4146000e-02 -1.1120000e-02 /
CHEB / -3.3612000e-02 -5.0876000e-02 -3.1527000e-02 /

CO+tSPC(1553)(+m)=CO2+C3H3O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #352 (C4H3O3J(1440))     deltaHrxn(T=298K) = -
29.327051914671557 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3168000e+00 -2.9949000e-11 -2.0740000e-11 /
CHEB / 2.9038000e+00 -5.2562000e-11 -3.6377000e-11 /
CHEB / -6.4907000e-01 -3.3722000e-11 -2.3285000e-11 /
CHEB / -9.0301000e-02 -1.1089000e-11 -7.5566000e-12 /
CHEB / 2.6240000e-02 7.2741000e-12 5.1914000e-12 /

sSPC(2810)+H2CCCO(+m)=CO+tSPC(1553)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #352 (C4H3O3J(1440))     deltaHrxn(T=298K) = -
56.29532150720479 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9766000e+00 -7.4359000e-01 -2.2901000e-01 /
CHEB / 1.0350000e+01 7.5691000e-01 1.7187000e-01 /
CHEB / -1.3335000e-01 1.1938000e-01 1.0413000e-01 /
CHEB / -1.3822000e-01 -6.6643000e-02 1.1591000e-03 /
CHEB / -7.9839000e-02 -6.2929000e-02 -3.2641000e-02 /

CO+tSPC(1553)(+m)=CO2+tSPC(346)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #352 (C4H3O3J(1440))    deltaHrxn(T=298K) = -
12.528813320518768 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9940000e+01 -7.4359000e-01 -2.2901000e-01 /
CHEB / 3.1360000e+01 7.5691000e-01 1.7187000e-01 /
CHEB / 1.3205000e-01 1.1938000e-01 1.0413000e-01 /
CHEB / -4.8682000e-02 -6.6643000e-02 1.1591000e-03 /
CHEB / -3.9558000e-02 -6.2929000e-02 -3.2641000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2              -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+H2CCCO(+m)=CO2+C3H3O-enone(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #696 (C4H3O3J(1458))     deltaHrxn(T=298K) = -
85.62237342187635 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2622000e+00 -1.2021000e-01 -7.4091000e-02 /
CHEB / 2.2115000e+00 1.2414000e-01 7.5054000e-02 /
CHEB / 1.7556000e-01 1.0733000e-02 7.4952000e-03 /
CHEB / 4.0730000e-02 -1.6849000e-02 -9.6222000e-03 /
CHEB / 8.5820000e-03 -4.7346000e-03 -3.2054000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2              -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!Here are the path reactions and their high-P limit kinetics:

CO+tSPC(1286)(+m)=CO2+tSPC(1553)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1153 (C4H3O4J(1450))    deltaHrxn(T=298K) = -
80.5315278208002 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7300000e+00 -3.0047000e-07 -2.0915000e-07 /
CHEB / 6.5953000e-01 -5.8938000e-07 -4.1025000e-07 /
CHEB / -6.3118000e-03 -5.5513000e-07 -3.8641000e-07 /
CHEB / 1.4219000e-03 -4.9952000e-07 -3.4771000e-07 /
CHEB / -4.5412000e-03 -4.2473000e-07 -2.9565000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     tBuOH       -75.1 78.01 27.2  34.21 40.27 45.3  53.28 59.16 68.42
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+HOC[CH2][CH3]2(+m)=CO2+tBuOH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1282 (C5H10O3(2367))
      deltaHrxn(T=298K) = -104.73938940619567 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0147000e+01 -1.4345000e+00 -3.2876000e-02 /
CHEB / 1.0769000e+00 9.7238000e-01 -3.7409000e-02 /
CHEB / 7.3338000e-02 5.8962000e-01 1.9776000e-02 /
CHEB / -4.1980000e-01 1.8426000e-01 5.3557000e-02 /
CHEB / -3.4122000e-01 -8.1161000e-02 3.9262000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+HCO(+m)=sSPC(2810)+iC4H7(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1418 (C5H8O2(1302))     deltaHrxn(T=298K) = -
30.096668401690856 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1861000e+01 -1.0522000e+00 -1.7404000e-01 /
CHEB / 5.6464000e-01 9.2504000e-01 5.9967000e-02 /
CHEB / 1.5025000e-01 2.7841000e-01 1.1096000e-01 /
CHEB / -6.3667000e-02 -2.8886000e-02 5.1976000e-02 /
CHEB / -7.4683000e-02 -7.9758000e-02 -9.2676000e-03 /

sSPC(2810)+iC4H7(+m)=C4H8O-i1+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1418 (C5H8O2(1302))     deltaHrxn(T=298K) = -
58.674342744989275 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2713000e+00 -1.4185000e+00 -5.5599000e-02 /
CHEB / 4.0948000e+00 9.6564000e-01 -6.0072000e-02 /
CHEB / 7.1550000e-01 5.3077000e-01 3.1214000e-02 /
CHEB / -8.1013000e-02 1.3756000e-01 7.2998000e-02 /
CHEB / -1.1436000e-01 -6.4743000e-02 4.9105000e-02 /

C4H7OJ(79)+HCO(+m)=C4H8O-i1+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1418 (C5H8O2(1302))    deltaHrxn(T=298K) = -
88.77101114668014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6005000e+00 -1.0570000e+00 -1.7690000e-01 /
CHEB / 1.7432000e+00 9.1886000e-01 6.0173000e-02 /
CHEB / 4.3536000e-01 2.8727000e-01 1.1121000e-01 /
CHEB / 4.5469000e-02 -2.2114000e-02 5.4599000e-02 /
CHEB / -2.8994000e-02 -7.9262000e-02 -7.2978000e-03 /

sSPC(2810)+iC4H7(+m)=CO2+iC4H8(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1418 (C5H8O2(1302))    deltaHrxn(T=298K) = -
91.84070184150302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0076000e+01 -1.4501000e+00 -5.1292000e-02 /
CHEB / 2.1348000e+00 9.3351000e-01 -6.0787000e-02 /
CHEB / 3.4946000e-01 5.5203000e-01 1.9324000e-02 /
CHEB / -1.7810000e-01 1.7991000e-01 6.5315000e-02 /
CHEB / -1.7037000e-01 -3.9487000e-02 5.4181000e-02 /
```

```
C4H7OJ(79)+HCO(+m)=CO2+iC4H8(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1418 (C5H8O2(1302))    deltaHrxn(T=298K) = -
121.93737024319387 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1598000e+01 -1.0582000e+00 -1.8417000e-01 /
CHEB / 5.1184000e-01 9.0766000e-01 6.2758000e-02 /
CHEB / 5.1390000e-02 2.9823000e-01 1.1336000e-01 /
CHEB / -7.9741000e-02 -1.2349000e-02 5.9037000e-02 /
CHEB / -7.4117000e-02 -7.8378000e-02 -4.5515000e-03 /

C4H8O-i1+CO(+m)=CO2+iC4H8(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1418 (C5H8O2(1302))    deltaHrxn(T=298K) = -
33.166359096513744 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5304000e+01 -1.4752000e+00 -4.7061000e-02 /
CHEB / 2.2316000e+01 9.0606000e-01 -6.0041000e-02 /
CHEB / 8.8409000e-01 5.6481000e-01 9.8883000e-03 /
CHEB / -2.2537000e-02 2.1153000e-01 5.7161000e-02 /
CHEB / -1.2495000e-01 -1.7375000e-02 5.5700000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+H2CCCH3[OH](+m)=CO2+iC4H8(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1578 (C5H8O2(1768))    deltaHrxn(T=298K) = -
47.69507814890801 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0904000e+01 -1.2367000e+00 -6.3959000e-02 /
CHEB / 1.7930000e+01 1.0944000e+00 -2.5272000e-02 /
```

```
CHEB / 3.7663000e-01 3.6098000e-01 7.4106000e-02 /
CHEB / -1.1741000e-01 -6.2373000e-02 5.2468000e-02 /
CHEB / -6.9461000e-02 -1.2990000e-01 -4.8321000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+CH2C[O]CH3(+m)=CO2+iC4H8(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1746 (C5H8O2(1769))    deltaHrxn(T=298K) = -
92.65059508065661 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1708000e+01 -1.1592000e+00 -9.2865000e-02 /
CHEB / 3.2118000e-01 1.0748000e+00 -9.8538000e-03 /
CHEB / -1.7544000e-01 2.6857000e-01 9.4387000e-02 /
CHEB / -1.8972000e-01 -8.2361000e-02 4.3205000e-02 /
CHEB / -5.2165000e-02 -9.8706000e-02 -1.3095000e-02 /

CH3CO+CH2C[O]CH3(+m)=CH2CO+H2CCCH3[OH](+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1746 (C5H8O2(1769))
      deltaHrxn(T=298K) = -44.95551693174859 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8405000e+00 -1.0633000e+00 -1.0541000e-01 /
CHEB / 1.8866000e+00 1.0696000e+00 1.9784000e-02 /
CHEB / 1.7816000e-01 1.8114000e-01 1.0046000e-01 /
CHEB / -3.7006000e-02 -1.1594000e-01 2.2299000e-02 /
CHEB / 6.7657000e-03 -8.8810000e-02 -2.3775000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+CH2C[O]CH3(+m)=CH2CO+H2CCCH3[OH](+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1922 (C5H8O2(2543))
      deltaHrxn(T=298K) = -53.52468708468743 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2862000e+00 -1.4551000e+00 -5.7140000e-02 /
CHEB / 2.4689000e+00 9.0710000e-01 -7.0936000e-02 /
CHEB / 4.2597000e-01 5.0159000e-01 9.5955000e-03 /
CHEB / -1.9981000e-01 1.3592000e-01 5.1658000e-02 /
CHEB / -1.7548000e-01 -4.8079000e-02 3.9790000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
sSPC(1590)+C2H3(+m)=CH2C[O]CH3+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2106 (C5H8O2(2898))     deltaHrxn(T=298K) = -
35.536894615436005 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2209000e+01 -5.4763000e-01 -2.2092000e-01 /
CHEB / 9.7344000e-02 4.6177000e-01 1.7005000e-01 /
CHEB / -5.9573000e-02 1.6828000e-01 6.9680000e-02 /
CHEB / -1.2530000e-01 -3.2088000e-02 3.2236000e-03 /
CHEB / -9.6250000e-02 -4.9659000e-02 -1.6927000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(213)+HCO(+m)=tSPC(77)+CO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2253 (C5H7O4J(3646))   deltaHrxn(T=298K) = -
44.80512183822896 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7196000e+00 -3.1274000e-03 -2.1725000e-03 /
CHEB / 1.0641000e+01 7.1914000e-06 6.5837000e-06 /
CHEB / 2.0439000e-01 -9.0963000e-04 -6.3025000e-04 /
CHEB / 6.2150000e-02 -8.1933000e-04 -5.6777000e-04 /
CHEB / 1.5391000e-02 -2.6623000e-04 -1.8397000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     iC4H7OJ(30) -10.03      77.94 24.19 29.26 33.77 37.63 43.83 48.46
      55.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!Here are the path reactions and their high-P limit kinetics:

iC4H7OJ(30)+H(+m)=iC4H8+O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2860 (C4H8OJJ(1751))   deltaHrxn(T=298K) =
16.77870213776489 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6473000e+00 -5.5555000e-03 -3.8548000e-03 /
CHEB / 7.4633000e+00 3.8589000e-03 2.6719000e-03 /
CHEB / 3.3373000e-01 -9.1837000e-04 -6.3465000e-04 /
CHEB / 1.3145000e-01 -8.1648000e-04 -5.6689000e-04 /
CHEB / 4.8411000e-02 -2.0336000e-04 -1.4162000e-04 /

C4H7OJ(79)+H(+m)=iC4H8+O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2860 (C4H8OJJ(1751))   deltaHrxn(T=298K) = -
6.948946845733367 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8133000e+00 -5.5188000e-03 -3.8293000e-03 /
CHEB / 2.6975000e+00 3.9292000e-03 2.7206000e-03 /
CHEB / 6.7494000e-01 -8.5632000e-04 -5.9158000e-04 /
CHEB / 2.0548000e-01 -7.6571000e-04 -5.3165000e-04 /
CHEB / 7.9431000e-02 -1.6489000e-04 -1.1493000e-04 /

C4H7OJ(79)+H(+m)=iC4H7OJ(30)+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2860 (C4H8OJJ(1751))   deltaHrxn(T=298K) = -
23.72764898349825 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0874000e+00 -5.5450000e-03 -3.8475000e-03 /
CHEB / -3.2040000e-01 3.8790000e-03 2.6858000e-03 /
CHEB / -1.0478000e-01 -9.0065000e-04 -6.2235000e-04 /
CHEB / -1.3662000e-02 -8.0193000e-04 -5.5679000e-04 /
CHEB / -7.3417000e-03 -1.9227000e-04 -1.3393000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
```

```
!     acetone     -51.56      70.09 17.97 22.0  25.89 29.34 34.93 39.15
      44.77 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

iC4H8+O(+m)=CH2+acetone(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3039 (C4H8OJJ(1752))   deltaHrxn(T=298K) = -
14.968490792161155 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7902000e+00 -1.5855000e-04 -1.1035000e-04 /
CHEB / 1.5293000e+00 5.0989000e-06 3.5513000e-06 /
CHEB / 2.2313000e-01 -1.9276000e-05 -1.3415000e-05 /
CHEB / 4.5412000e-02 -4.4206000e-05 -3.0765000e-05 /
CHEB / 3.2051000e-03 -1.5072000e-05 -1.0489000e-05 /

iC4H8+O(+m)=CH2C[O]CH3+CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3039 (C4H8OJJ(1752))   deltaHrxn(T=298K) = -
23.847720467134955 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1305000e+01 -1.7252000e-04 -1.2007000e-04 /
CHEB / 8.2331000e-01 -2.1071000e-06 -1.4628000e-06 /
CHEB / 2.6986000e-03 -1.4525000e-05 -1.0108000e-05 /
CHEB / -3.2197000e-03 -4.5072000e-05 -3.1368000e-05 /
CHEB / -1.0130000e-02 -1.6836000e-05 -1.1716000e-05 /

CH2+acetone(+m)=CH2C[O]CH3+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3039 (C4H8OJJ(1752))   deltaHrxn(T=298K) = -8.8792296749738
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0266000e+01 -1.0558000e-03 -7.3421000e-04 /
CHEB / 1.7257000e+00 1.0002000e-03 6.9537000e-04 /
CHEB / 4.9780000e-02 -6.1871000e-05 -4.3047000e-05 /
CHEB / 1.6988000e-02 -2.4250000e-04 -1.6854000e-04 /
CHEB / 6.9509000e-03 3.1932000e-05 2.2153000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     iC4H7OJ(17) -2.16 80.25 24.19 29.61 34.26 38.15 44.29 48.75 55.48
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+sC3H5=C4H7OJ(79)   3.2847733e+07      1.50370
7.3354000e+03
!     C4H6Oi-13+H=C4H7OJ(79)  1.0000000e+11      0.00000
1.1900000e+04
!     tSPC(110)+H=C4H7OJ(79)  1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7OJ(79)=iC4H7OJ(15)  8.1282219e+08      1.13906
3.4790987e+04
!     C4H7OJ(79)=iC4H7OJ(17)  9.0000000e+11      0.00000
2.9400000e+04
!     O+iC4H7=C4H7OJ(79)      1.0000000e+13      0.00000
0.0000000e+00

CH2+CH2C[O]CH3(+m)=C4H7OJ(79)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
75.7220051188167 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0034000e+00 9.1120000e+00 -8.3887000e-01 /
CHEB / -4.6021000e+00 1.2454000e+00 7.8356000e-01 /
CHEB / -4.0329000e+00 -1.8560000e-01 6.3991000e-01 /
CHEB / -2.0575000e+00 -5.6933000e-01 2.3731000e-01 /
CHEB / -8.7575000e-01 -4.1022000e-01 1.3891000e-02 /

iC4H7+O(+m)=C4H7OJ(79)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200)) High-P Limit: Oa_R_Recombination
estimate: (Average:) Oa     C_rad/H2/Cd         deltaHrxn(T=298K) = -
78.14186293522036 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3383000e+00 8.5422000e+00 -9.0881000e-01 /
CHEB / -5.9763000e+00 1.3811000e+00 8.0667000e-01 /
CHEB / -4.0384000e+00 -1.1944000e-01 6.4009000e-01 /
CHEB / -2.0786000e+00 -5.6029000e-01 2.4023000e-01 /
CHEB / -8.7765000e-01 -4.2317000e-01 2.3540000e-02 /
```

```
iC4H7+O(+m)=CH2+CH2C[O]CH3(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
2.419857816403673 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5231000e+00 -4.1028000e-02 -2.7345000e-02 /
CHEB / 3.1212000e+00 5.0428000e-02 3.3375000e-02 /
CHEB / 5.6267000e-01 -4.3656000e-03 -2.5530000e-03 /
CHEB / 1.2871000e-01 -5.3042000e-03 -3.5950000e-03 /
CHEB / 2.1327000e-02 -8.6157000e-04 -6.5524000e-04 /

CH2O+sC3H5(+m)=C4H7OJ(79)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H2_O     Cd_rad/NonDe         deltaHrxn(T=298K)
= -21.897732295261925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2412000e+00 1.1100000e+00 -1.3695000e-01 /
CHEB / -2.1809000e+00 9.0470000e-01 1.2419000e-01 /
CHEB / -2.8609000e+00 1.8595000e-01 4.1867000e-02 /
CHEB / -1.4280000e+00 -1.2138000e-01 -1.0146000e-02 /
CHEB / -5.4202000e-01 -1.1185000e-01 -1.8097000e-02 /

CH2+CH2C[O]CH3(+m)=CH2O+sC3H5(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
53.824272823554764 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3457000e+00 5.2193000e-02 2.9122000e-02 /
CHEB / 1.8227000e+00 -4.4306000e-02 -2.2411000e-02 /
CHEB / -1.2563000e-01 -1.4818000e-02 -9.1495000e-03 /
CHEB / -5.0255000e-02 -1.8260000e-05 -2.8530000e-03 /
CHEB / -1.7264000e-02 3.9418000e-03 2.2679000e-03 /

iC4H7+O(+m)=CH2O+sC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
56.24413063995844 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3771000e+01 1.9497000e-05 1.1610000e-05 /
CHEB / -6.1875000e-01 1.1889000e-05 9.0349000e-06 /
CHEB / 4.4942000e-03 -2.1044000e-05 -1.1767000e-05 /
CHEB / 1.4262000e-02 -2.2065000e-05 -1.5834000e-05 /
CHEB / 8.2855000e-03 -4.3610000e-06 -5.0936000e-06 /

C4H6Oi-13+H(+m)=CH2+CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = 67.7634435596953
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9085000e+01 1.0359000e-01 6.2188000e-02 /
CHEB / 2.3948000e+01 -8.2540000e-02 -4.4622000e-02 /
CHEB / -2.9926000e-01 -3.2393000e-02 -2.1134000e-02 /
CHEB / -8.5818000e-02 -3.6121000e-03 -8.0211000e-03 /
CHEB / -1.3475000e-02 4.1863000e-03 1.6095000e-03 /
```

```
iC4H7+O(+m)=C4H6Oi-13+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -70.183301376099
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1979000e+00 1.6306000e-04 1.1245000e-04 /
CHEB / -2.0253000e+00 -7.2648000e-05 -4.7382000e-05 /
CHEB / -4.1440000e-01 -7.6043000e-05 -5.0054000e-05 /
CHEB / -1.3680000e-01 -5.3457000e-05 -4.1646000e-05 /
CHEB / -5.0828000e-02 -1.4036000e-05 -1.5281000e-05 /

C4H6Oi-13+H(+m)=CH2O+sC3H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) =
13.939170736140547 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0412000e+00 -7.3530000e-01 -1.2829000e-01 /
CHEB / 5.8070000e+00 8.6558000e-01 1.3072000e-01 /
CHEB / -4.0053000e-01 1.0195000e-02 2.6990000e-02 /
CHEB / -4.5972000e-02 -1.3726000e-01 -1.8854000e-02 /
CHEB / 6.9122000e-02 -4.0645000e-02 -1.5322000e-02 /

tSPC(110)+H(+m)=C4H7OJ(79)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200)) High-P Limit: R_Recombination estimate:
(Average:) Y_rad     H_rad          deltaHrxn(T=298K) = -
61.363160837102065 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2386000e+00 5.8082000e+00 -3.0910000e-01 /
CHEB / -5.3365000e+00 5.8086000e-01 -6.5001000e-03 /
CHEB / -3.4351000e+00 -9.2341000e-03 4.7195000e-01 /
CHEB / -1.6524000e+00 -4.2098000e-01 3.8999000e-01 /
CHEB / -6.2286000e-01 -4.2746000e-01 1.7489000e-01 /

tSPC(110)+H(+m)=CH2+CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) =
14.358844281714628 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3397000e-01 -3.9288000e-02 -2.7749000e-02 /
CHEB / 7.4726000e+00 4.4794000e-02 3.1648000e-02 /
CHEB / 3.6460000e-01 1.9769000e-03 1.3538000e-03 /
CHEB / 1.1308000e-01 -7.7089000e-03 -5.3736000e-03 /
CHEB / 4.1596000e-02 -9.5085000e-04 -7.0853000e-04 /

tSPC(110)+H(+m)=iC4H7+O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) =
16.778702098118295 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5964000e+00 -5.6552000e-04 -3.9330000e-04 /
CHEB / 6.4903000e+00 6.5874000e-04 4.5819000e-04 /
CHEB / 7.6447000e-01 -1.4811000e-05 -1.0508000e-05 /
CHEB / 2.7173000e-01 -7.8853000e-05 -5.4678000e-05 /
CHEB / 1.0691000e-01 -7.8261000e-06 -5.3645000e-06 /
```

```
tSPC(110)+H(+m)=CH2O+sC3H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
39.46542854184014 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2893000e+01 -3.5129000e-07 -2.7265000e-07 /
CHEB / -1.2371000e-01 4.3863000e-07 3.3961000e-07 /
CHEB / 1.2248000e-02 5.9290000e-09 1.6470000e-09 /
CHEB / 5.9437000e-02 -9.7899000e-08 -7.4128000e-08 /
CHEB / 3.9346000e-02 -1.9498000e-08 -1.0538000e-08 /

tSPC(110)+H(+m)=C4H6Oi-13+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4590000e+00 5.8362000e-04 4.0868000e-04 /
CHEB / -1.6045000e+00 -6.2527000e-04 -4.3821000e-04 /
CHEB / -4.3526000e-01 -6.5260000e-05 -4.5384000e-05 /
CHEB / -9.8396000e-02 9.3295000e-05 6.5557000e-05 /
CHEB / -2.0938000e-02 2.7329000e-05 1.9032000e-05 /

CH2+CH2C[O]CH3(+m)=iC4H7OJ(15)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
99.24972451530242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4226000e+00 2.9470000e-02 1.4482000e-02 /
CHEB / 2.9358000e+00 -2.4622000e-02 -1.0249000e-02 /
CHEB / 1.9829000e-01 -8.2947000e-03 -4.8488000e-03 /
CHEB / 6.4472000e-02 -9.2394000e-04 -2.6895000e-03 /
CHEB / 2.7188000e-02 2.5447000e-03 1.4595000e-03 /

iC4H7+O(+m)=iC4H7OJ(15)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
101.6695823317061 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8325000e+00 -6.7795000e-05 -4.8977000e-05 /
CHEB / 5.1155000e-01 8.6534000e-05 6.0615000e-05 /
CHEB / 3.3644000e-01 6.6364000e-07 2.8875000e-06 /
CHEB / 1.3185000e-01 -2.2277000e-05 -1.5433000e-05 /
CHEB / 5.3607000e-02 -6.7002000e-06 -6.0018000e-06 /

C4H6Oi-13+H(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
31.48628095560711 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0590000e-01 -2.7104000e-01 -1.5435000e-01 /
CHEB / 8.5266000e+00 3.4795000e-01 1.9122000e-01 /
CHEB / -2.7324000e-02 -2.8174000e-02 -7.4783000e-03 /
CHEB / 9.0893000e-02 -6.3508000e-02 -3.3804000e-02 /
CHEB / 9.0782000e-02 -3.3487000e-03 -5.6012000e-03 /
```

```
tSPC(110)+H(+m)=iC4H7OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
84.8908802335878 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8422000e+00 -4.0526000e-04 -2.8305000e-04 /
CHEB / 1.0731000e+00 4.5824000e-04 3.2019000e-04 /
CHEB / 3.6650000e-01 1.8205000e-05 1.2556000e-05 /
CHEB / 1.8062000e-01 -7.0704000e-05 -4.9443000e-05 /
CHEB / 8.4722000e-02 -1.1438000e-05 -7.9234000e-06 /

CH2O+sC3H5(+m)=iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
45.425451691747654 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7179000e+00 -2.6309000e-01 -1.2600000e-01 /
CHEB / 5.6547000e+00 3.5211000e-01 1.6346000e-01 /
CHEB / 4.1239000e-01 -6.1173000e-02 -2.1163000e-02 /
CHEB / 1.6076000e-01 -4.4477000e-02 -2.1869000e-02 /
CHEB / 9.1328000e-02 9.3720000e-03 9.0606000e-04 /

CH2+CH2C[O]CH3(+m)=iC4H7OJ(17)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
91.58043062309832 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8202000e+00 5.2193000e-02 2.9122000e-02 /
CHEB / 2.2588000e+00 -4.4306000e-02 -2.2411000e-02 /
CHEB / -1.1002000e-02 -1.4818000e-02 -9.1495000e-03 /
CHEB / -1.0099000e-02 -1.8260000e-05 -2.8530000e-03 /
CHEB / -1.4577000e-03 3.9418000e-03 2.2679000e-03 /

iC4H7+O(+m)=iC4H7OJ(17)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -94.000288439502
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0246000e+01 1.9497000e-05 1.1610000e-05 /
CHEB / -1.8260000e-01 1.1889000e-05 9.0349000e-06 /
CHEB / 1.1912000e-01 -2.1044000e-05 -1.1767000e-05 /
CHEB / 5.4418000e-02 -2.2065000e-05 -1.5834000e-05 /
CHEB / 2.4092000e-02 -4.3610000e-06 -5.0936000e-06 /

CH2O+sC3H5(+m)=iC4H7OJ(17)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
37.75615779954356 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4191000e+00 -5.5281000e-01 -1.2042000e-01 /
CHEB / 3.7375000e+00 7.2809000e-01 1.3310000e-01 /
CHEB / 1.9628000e-01 -1.1700000e-01 1.6216000e-02 /
CHEB / 7.8535000e-02 -7.9958000e-02 -2.5072000e-02 /
CHEB / 7.9270000e-02 4.6017000e-03 -1.2619000e-02 /
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```
C4H6Oi-13+H(+m)=iC4H7OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
23.816987063403012 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.5157000e+00 -7.3530000e-01 -1.2829000e-01 /
CHEB / 6.2432000e+00 8.6558000e-01 1.3072000e-01 /
CHEB / -2.8591000e-01 1.0195000e-02 2.6990000e-02 /
CHEB / -5.8157000e-03 -1.3726000e-01 -1.8854000e-02 /
CHEB / 8.4929000e-02 -4.0645000e-02 -1.5322000e-02 /

tSPC(110)+H(+m)=iC4H7OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3147 (C4H7OJ(1200))    deltaHrxn(T=298K) = -
77.2215863413837 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3670000e+00 -3.5129000e-07 -2.7265000e-07 /
CHEB / 3.1243000e-01 4.3863000e-07 3.3961000e-07 /
CHEB / 1.2687000e-01 5.9290000e-09 1.6470000e-09 /
CHEB / 9.9593000e-02 -9.7899000e-08 -7.4128000e-08 /
CHEB / 5.5153000e-02 -1.9498000e-08 -1.0538000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(213)+O(+m)=tSPC(3683)+HCO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3385 (C4H6O4JJ(3659))  deltaHrxn(T=298K) = -
24.717341266878748 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0657000e+01 3.0253000e-09 2.1056000e-09 /
CHEB / 1.3610000e+00 1.1097000e-08 7.7244000e-09 /
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CHEB / -2.1778000e-02 1.0096000e-08 7.0273000e-09 /
CHEB / -2.8865000e-02 5.6690000e-09 3.9460000e-09 /
CHEB / -3.4984000e-02 2.0529000e-09 1.4290000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1590)+H(+m)=H2CCCH3[OH]+O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3859 (C3H6O2JJ(2484))  deltaHrxn(T=298K) =
4.439325973382992 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5393000e+00 -5.8173000e-03 -4.0355000e-03 /
CHEB / 3.7846000e+00 4.2761000e-03 2.9601000e-03 /
CHEB / 4.9443000e-01 -8.5470000e-04 -5.9000000e-04 /
CHEB / 1.3218000e-01 -8.4114000e-04 -5.8395000e-04 /
CHEB / 3.2444000e-02 -2.5808000e-04 -1.7968000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

H2CCCH3[OH]+O(+m)=CH2C[O]CH3+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4062 (C3H6O2JJ(2485))  deltaHrxn(T=298K) = -
14.328714708355998 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 6.7289000e+00 -3.5030000e-06 -2.4383000e-06 /
CHEB / 3.9619000e+00 -6.5187000e-06 -4.5375000e-06 /
CHEB / 1.2150000e-01 -5.2851000e-06 -3.6788000e-06 /
CHEB / 3.5940000e-02 -3.7766000e-06 -2.6288000e-06 /
CHEB / 7.1990000e-03 -2.3939000e-06 -1.6663000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CO            -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

H2CCCO+O(+m)=CO+CH2CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4942 (C3H2O2JJ(1578))  deltaHrxn(T=298K) = -
137.75697276965062 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0520000e+01 -4.6102000e-08 -3.2091000e-08 /
CHEB / 1.5269000e+00 -9.0357000e-08 -6.2895000e-08 /
CHEB / 4.9510000e-03 -8.4909000e-08 -5.9103000e-08 /
CHEB / -5.8202000e-04 -7.6140000e-08 -5.2999000e-08 /
CHEB / -1.3626000e-02 -6.4474000e-08 -4.4879000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2O               75.16 57.47 12.08 13.91 15.4  16.64 18.61 20.1
      22.47 null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!Here are the path reactions and their high-P limit kinetics:

H2CCCO+O(+m)=C2O+CH2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5625 (C3H2O2JJ(1577))  deltaHrxn(T=298K) = -
50.79594117529575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0728000e+01 2.8804000e-12 2.0036000e-12 /
CHEB / 1.4221000e+00 5.6315000e-12 3.9231000e-12 /
CHEB / 5.0591000e-02 5.2685000e-12 3.6649000e-12 /
CHEB / 3.9107000e-02 4.6854000e-12 3.2636000e-12 /
CHEB / 2.2631000e-02 3.9335000e-12 2.7364000e-12 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(77)+O(+m)=tSPC(213)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6369 (C4H7O3J(4117))   deltaHrxn(T=298K) = -
70.18330155923155 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4491000e+00 6.6414000e-04 4.6503000e-04 /
CHEB / -2.2481000e+00 -7.4087000e-04 -5.1929000e-04 /
CHEB / -4.5979000e-01 -2.0579000e-05 -1.3763000e-05 /
CHEB / -1.5735000e-01 7.8987000e-05 5.5384000e-05 /
```

```
CHEB / -5.6779000e-02 2.8524000e-05 1.9815000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+H2O(+m)=CH2O+CH3C[OH]CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6712 (C4H9O2J(1755))    deltaHrxn(T=298K) = -
4.949323379773752 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9431000e+00 1.3921000e-07 9.4552000e-08 /
CHEB / 1.6722000e+01 6.0220000e-07 4.2031000e-07 /
CHEB / 2.7784000e-01 3.8158000e-07 2.6839000e-07 /
CHEB / 8.6393000e-02 1.4411000e-07 9.9599000e-08 /
CHEB / 9.7806000e-03 7.6870000e-08 5.1966000e-08 /

O+HOC[CH2][CH3]2(+m)=CH2O+CH3C[OH]CH3(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6712 (C4H9O2J(1755))    deltaHrxn(T=298K) = -
82.4916445621049 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3918000e+01 4.0676000e-07 2.8313000e-07 /
CHEB / -8.6995000e-01 8.1263000e-07 5.6565000e-07 /
CHEB / -7.8830000e-02 6.6133000e-07 4.6033000e-07 /
CHEB / -6.1279000e-02 4.7162000e-07 3.2828000e-07 /
CHEB / -5.6327000e-02 3.1080000e-07 2.1634000e-07 /
```

```
O+HOC[CH2][CH3]2(+m)=C4H7OJ(79)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6712 (C4H9O2J(1755))    deltaHrxn(T=298K) = -
77.54232118233114 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4110000e+00 -1.9133000e-04 -1.3317000e-04 /
CHEB / 2.3544000e+00 1.2137000e-04 8.4481000e-05 /
CHEB / 1.0141000e+00 9.2063000e-05 6.4078000e-05 /
CHEB / 2.9521000e-01 1.4395000e-06 1.0025000e-06 /
CHEB / 4.7240000e-02 -1.8147000e-05 -1.2630000e-05 /

iC4H8+HO2(+m)=CH2O+CH3C[OH]CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6712 (C4H9O2J(1755))   deltaHrxn(T=298K) = -
45.67551815260312 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7568000e+00 -4.8310000e-01 -1.8185000e-01 /
CHEB / 6.9744000e+00 5.8586000e-01 1.9593000e-01 /
CHEB / -1.4481000e-01 -1.9215000e-02 2.9971000e-02 /
CHEB / -2.1187000e-01 -8.6572000e-02 -3.4900000e-02 /
CHEB / -1.5625000e-01 -2.2071000e-02 -2.1488000e-02 /

iC4H8+HO2(+m)=C4H7OJ(79)+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6712 (C4H9O2J(1755))   deltaHrxn(T=298K) = -
40.72619477282937 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.6733000e+00 -3.7427000e-01 -1.6034000e-01 /
CHEB / 1.0799000e+01 4.9160000e-01 1.9217000e-01 /
CHEB / 9.8878000e-01 -7.2237000e-02 1.5498000e-03 /
CHEB / 1.0898000e-01 -6.1746000e-02 -3.6036000e-02 /
CHEB / -7.6224000e-02 1.5281000e-03 -8.0861000e-03 /

O+HOC[CH2][CH3]2(+m)=iC4H8+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6712 (C4H9O2J(1755))   deltaHrxn(T=298K) = -
36.81612640950177 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4955000e+00 -6.8788000e-02 -5.1065000e-02 /
CHEB / 2.4270000e+00 9.3353000e-02 6.8280000e-02 /
CHEB / 7.5196000e-01 -1.6824000e-02 -1.0648000e-02 /
CHEB / 4.0655000e-02 -1.2264000e-02 -9.7360000e-03 /
CHEB / -9.8373000e-02 2.0419000e-03 9.8865000e-04 /

C4H8O2(62)+H(+m)=CH2O+CH3C[OH]CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6712 (C4H9O2J(1755))    deltaHrxn(T=298K) = -
75.98177761475343 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1083000e+01 -1.6175000e-01 -9.8930000e-02 /
CHEB / 8.9607000e-01 1.9209000e-01 1.1458000e-01 /
CHEB / 4.1529000e-02 -1.9337000e-03 3.0139000e-03 /
CHEB / -1.1396000e-01 -2.9012000e-02 -1.7697000e-02 /
CHEB / -1.2173000e-01 -6.4036000e-03 -5.5508000e-03 /
```

```
C4H8O2(62)+H(+m)=C4H7OJ(79)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6712 (C4H9O2J(1755))   deltaHrxn(T=298K) = -
71.03245423497967 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4713000e+00 -1.6265000e-01 -9.6068000e-02 /
CHEB / 4.1823000e+00 1.9860000e-01 1.1417000e-01 /
CHEB / 1.0634000e+00 -1.1593000e-02 -2.2060000e-03 /
CHEB / 1.9015000e-01 -2.7149000e-02 -1.6376000e-02 /
CHEB / -3.2273000e-02 -2.7104000e-03 -3.0876000e-03 /

C4H8O2(62)+H(+m)=O+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #6712 (C4H9O2J(1755))    deltaHrxn(T=298K) =
6.5098669473514725 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.7359000e-01 -1.0147000e-01 -6.3605000e-02 /
CHEB / 6.7007000e+00 1.2940000e-01 7.9561000e-02 /
CHEB / 1.2458000e+00 -1.6762000e-02 -7.9298000e-03 /
CHEB / 1.6785000e-01 -1.3679000e-02 -9.2929000e-03 /
CHEB / -4.6279000e-02 4.3847000e-05 -4.9702000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     C2H3O-2           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     CH2CO+H=CH2CHO          3.4049294e+12      0.23000
3.1333333e+03
!     CH2CHO=CH3CO            2.0320555e+08      1.13906
3.4790987e+04
!     CH2CO+H=CH3CO           1.8833259e+13      0.00000
2.9000000e+03
!     CH3+CO=CH3CO            5.0600000e+11      0.00000
6.8800000e+03
```

```
!     CH2CHO=C2H3O-1                8.1282219e+08      1.13906
3.4790987e+04
!     CH2CHO=C2H3O-2                2.0320555e+08      1.13906
3.4790987e+04
!     C2H3+O=CH2CHO           1.0000000e+13      0.00000
0.0000000e+00

CH2CHO(+m)=CH3CO(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_2H     CO_H_out       deltaHrxn(T=298K) = -
8.569170152938833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7565000e+01 5.1785000e+00 6.5284000e-01 /
CHEB / 1.1383000e+01 -7.3274000e-01 -1.6851000e-01 /
CHEB / -5.8093000e-01 -5.7031000e-01 -3.1745000e-02 /
CHEB / -5.5813000e-01 -1.4053000e-01 5.0821000e-02 /
CHEB / -5.2041000e-01 1.5675000e-01 5.4248000e-02 /

CH2CO+H(+m)=CH3CO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Cd/H2_Ck     H_rad       deltaHrxn(T=298K) = -
39.93536336144922 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8312000e+00 4.9008000e+00 8.3153000e-01 /
CHEB / 1.0727000e+00 -1.0145000e+00 -1.4998000e-01 /
CHEB / -1.6721000e-01 -7.3850000e-01 -4.5121000e-02 /
CHEB / -2.8876000e-01 -2.3650000e-01 4.9955000e-02 /
CHEB / -3.7543000e-01 1.0415000e-01 6.5748000e-02 /

CH2CO+H(+m)=CH3+CO(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -29.26703133357845 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2272000e+01 -1.1864000e-02 2.1444000e-03 /
CHEB / 9.4515000e-01 -4.9896000e-04 -4.2672000e-03 /
CHEB / 3.0873000e-02 1.0331000e-02 -1.7022000e-03 /
CHEB / 5.7770000e-02 6.2204000e-03 2.8412000e-03 /
CHEB / 3.0440000e-02 1.0487000e-04 2.6606000e-03 /

C2H3+O(+m)=CH2CHO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO) High-P Limit: Oa_R_Recombination estimate: (Average:)
Cd_pri_rad     Oa       deltaHrxn(T=298K) = -124.86710088201681 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1986000e+01 1.7096000e+01 1.6666000e+00 /
CHEB / -7.4842000e+00 -4.4816000e+00 1.0179000e+00 /
CHEB / -1.8140000e+00 -1.9980000e+00 -9.1588000e-01 /
CHEB / -6.0638000e-01 -6.1304000e-01 -4.2382000e-01 /
CHEB / -2.8559000e-01 -1.8677000e-01 -3.3609000e-02 /

C2H3+O(+m)=CH3CO(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -133.43627103495564 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5561000e+01 1.5989000e+01 4.0941000e+00 /
```

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CHEB / -5.6044000e+00 -4.3108000e+00 2.3393000e-01 /
CHEB / -1.6447000e+00 -1.5396000e+00 -1.1007000e+00 /
CHEB / -6.0116000e-01 -5.0308000e-01 -4.6983000e-01 /
CHEB / -3.4275000e-01 -1.9495000e-01 2.1002000e-02 /

C2H3+O(+m)=CH2CO+H(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -93.50090767350645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6501000e+00 -1.2249000e-03 -9.3356000e-04 /
CHEB / -2.8130000e+00 1.7846000e-03 1.3816000e-03 /
CHEB / -5.8820000e-01 -7.0925000e-04 -5.8234000e-04 /
CHEB / -1.8522000e-01 2.0534000e-04 1.8388000e-04 /
CHEB / -6.9641000e-02 -7.0099000e-05 -6.1353000e-05 /

C2H3+O(+m)=CH3+CO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -122.76793900708488 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2882000e+01 -3.0113000e-04 -2.6970000e-04 /
CHEB / -5.5083000e-01 5.5279000e-04 4.9167000e-04 /
CHEB / -3.4990000e-03 -3.9412000e-04 -3.4876000e-04 /
CHEB / 1.4764000e-02 2.0995000e-04 1.8518000e-04 /
CHEB / 6.5040000e-03 -7.7897000e-05 -6.8060000e-05 /

CH2CHO(+m)=C2H3O-1(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO) High-P Limit: intra_H_migration estimate: (Average:)
R3H_SD     O_rad_out     Cd_H_out_singleH       deltaHrxn(T=298K) =
23.197518509291335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0162000e+00 6.2105000e-01 -7.2844000e-02 /
CHEB / 1.0594000e+01 9.1703000e-01 -3.8112000e-02 /
CHEB / -9.5812000e-01 4.2111000e-01 5.1261000e-02 /
CHEB / -5.7938000e-01 9.2750000e-02 5.2679000e-02 /
CHEB / -3.0161000e-01 -3.1388000e-02 1.7899000e-02 /

CH3CO(+m)=C2H3O-1(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = 31.766688662230166 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3158000e+01 3.5591000e+00 6.7229000e-01 /
CHEB / 1.6327000e+01 -1.6028000e-01 -1.1685000e-01 /
CHEB / 1.3970000e-01 -3.3699000e-01 3.2605000e-02 /
CHEB / -3.2290000e-01 -1.2993000e-01 9.6194000e-02 /
CHEB / -4.4015000e-01 9.9017000e-02 6.9022000e-02 /

CH2CO+H(+m)=C2H3O-1(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -8.16867469921905 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0833000e+01 -1.0899000e+00 -1.1840000e-01 /
CHEB / 2.2680000e+00 1.0517000e+00 1.4735000e-02 /
CHEB / 1.0422000e-01 2.1722000e-01 1.1220000e-01 /
CHEB / -3.3431000e-02 -8.5726000e-02 3.9097000e-02 /
CHEB / -2.6546000e-03 -8.1512000e-02 -2.0885000e-02 /
```

```
CH3+CO(+m)=C2H3O-1(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = 21.0983566343594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5109000e+00 -1.1457000e+00 -9.9587000e-02 /
CHEB / 1.3521000e+01 1.0736000e+00 -7.5967000e-03 /
CHEB / 4.4536000e-01 2.5602000e-01 1.0504000e-01 /
CHEB / 6.7517000e-02 -7.6869000e-02 4.7509000e-02 /
CHEB / 4.8079000e-02 -8.7236000e-02 -1.5526000e-02 /

C2H3+O(+m)=C2H3O-1(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -101.66958237272549 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3490000e+01 -3.1393000e-04 -2.7862000e-04 /
CHEB / -5.3961000e-01 5.5869000e-04 4.9578000e-04 /
CHEB / 5.0022000e-03 -3.8941000e-04 -3.4545000e-04 /
CHEB / 2.0969000e-02 2.0993000e-04 1.8514000e-04 /
CHEB / 1.0896000e-02 -7.8499000e-05 -6.8476000e-05 /

CH2CHO(+m)=C2H3O-2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    O_rad_out     Cd_H_out_doubleC        deltaHrxn(T=298K)
= 23.197518509291335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.6183000e+00 6.2105000e-01 -7.2844000e-02 /
CHEB / 1.0594000e+01 9.1703000e-01 -3.8112000e-02 /
CHEB / -9.5812000e-01 4.2111000e-01 5.1261000e-02 /
CHEB / -5.7938000e-01 9.2750000e-02 5.2679000e-02 /
CHEB / -3.0161000e-01 -3.1388000e-02 1.7899000e-02 /

CH3CO(+m)=C2H3O-2(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = 31.766688662230166 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3760000e+01 3.5591000e+00 6.7229000e-01 /
CHEB / 1.6327000e+01 -1.6028000e-01 -1.1685000e-01 /
CHEB / 1.3970000e-01 -3.3699000e-01 3.2605000e-02 /
CHEB / -3.2290000e-01 -1.2993000e-01 9.6194000e-02 /
CHEB / -4.4015000e-01 9.9017000e-02 6.9022000e-02 /

CH2CO+H(+m)=C2H3O-2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -8.16867469921905 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0231000e+01 -1.0899000e+00 -1.1840000e-01 /
CHEB / 2.2680000e+00 1.0517000e+00 1.4735000e-02 /
CHEB / 1.0422000e-01 2.1722000e-01 1.1220000e-01 /
CHEB / -3.3431000e-02 -8.5726000e-02 3.9097000e-02 /
CHEB / -2.6546000e-03 -8.1512000e-02 -2.0885000e-02 /

CH3+CO(+m)=C2H3O-2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = 21.0983566343594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1129000e+00 -1.1457000e+00 -9.9587000e-02 /
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CHEB / 1.3521000e+01 1.0736000e+00 -7.5967000e-03 /
CHEB / 4.4536000e-01 2.5602000e-01 1.0504000e-01 /
CHEB / 6.7517000e-02 -7.6869000e-02 4.7509000e-02 /
CHEB / 4.8079000e-02 -8.7236000e-02 -1.5526000e-02 /

C2H3+O(+m)=C2H3O-2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#7154 (CH2CHO)    deltaHrxn(T=298K) = -101.66958237272549 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2888000e+01 -3.1393000e-04 -2.7862000e-04 /
CHEB / -5.3961000e-01 5.5869000e-04 4.9578000e-04 /
CHEB / 5.0022000e-03 -3.8941000e-04 -3.4545000e-04 /
CHEB / 2.0969000e-02 2.0993000e-04 1.8514000e-04 /
CHEB / 1.0896000e-02 -7.8499000e-05 -6.8476000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     HCOOH       -90.2 59.4  10.83 12.87 14.62 15.98 18.4  20.0  20.0
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

C2H4O+O(+m)=CH2+HCOOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7758 (C2H4O2JJ(801))   deltaHrxn(T=298K) = -
27.79732229013449 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0305000e+01 -9.6820000e-05 -6.7391000e-05 /
CHEB / 1.5557000e+00 -6.6343000e-06 -4.6171000e-06 /
CHEB / -2.2883000e-02 -8.1620000e-06 -5.6806000e-06 /
CHEB / -1.6553000e-02 -1.9014000e-05 -1.3234000e-05 /
CHEB / -1.3978000e-02 -1.4127000e-05 -9.8322000e-06 /

C2H4O+O(+m)=CH2CHO+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7758 (C2H4O2JJ(801))   deltaHrxn(T=298K) = -14.328714867316
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5373000e+00 -9.4504000e-05 -6.5779000e-05 /
CHEB / 1.9738000e+00 -3.6351000e-06 -2.5297000e-06 /
CHEB / 1.3713000e-01 -6.8688000e-06 -4.7806000e-06 /
CHEB / 4.2568000e-02 -1.8334000e-05 -1.2760000e-05 /
```

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CHEB / 6.2181000e-03 -1.3654000e-05 -9.5035000e-06 /

CH2CHO+OH(+m)=CH2+HCOOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7758 (C2H4O2JJ(801))   deltaHrxn(T=298K) = -
13.468607422818494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3095000e+01 -3.2638000e-04 -2.2714000e-04 /
CHEB / -6.8936000e-01 1.5258000e-04 1.0618000e-04 /
CHEB / -5.6389000e-02 3.6806000e-05 2.5612000e-05 /
CHEB / -2.3061000e-02 -4.3535000e-05 -3.0294000e-05 /
CHEB / -1.8886000e-02 -2.8894000e-05 -2.0107000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

CH3O+C2H3(+m)=CH3+CH2CHO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8003 (C3H6O(1390))     deltaHrxn(T=298K) = -
34.686900937162385 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2838000e+01 -6.5143000e-03 -5.4598000e-03 /
CHEB / -1.5229000e-01 3.2628000e-03 2.7716000e-03 /
CHEB / -1.9364000e-02 5.7209000e-03 4.7606000e-03 /
CHEB / 5.6104000e-03 -7.5007000e-04 -6.5978000e-04 /
CHEB / -1.0853000e-03 -1.9572000e-03 -1.6216000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     CO2              -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     iC4H9       16.5  76.33 22.57 28.26 33.45 37.96 45.1  50.52 60.07
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+iC4H8(+m)=CO+HOC[CH2][CH3]2(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #8310 (C5H9O2J(2258))
      deltaHrxn(T=298K) = -10.419265802495037 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9221000e+00 -1.4990000e-01 -1.0335000e-01 /
CHEB / 1.6178000e+01 1.3010000e-01 8.9267000e-02 /
CHEB / 3.2968000e-01 5.7568000e-02 3.8075000e-02 /
CHEB / 1.4353000e-02 -1.6117000e-02 -8.3536000e-03 /
CHEB / -5.2347000e-02 -1.9692000e-02 -1.2708000e-02 /

sSPC(2810)+iC4H8(+m)=CO2+iC4H9(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8310 (C5H9O2J(2258))   deltaHrxn(T=298K) = -
35.44635229816337 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.3486000e+00 -1.9263000e-01 -1.2534000e-01 /
CHEB / 1.4452000e+01 1.7181000e-01 1.1019000e-01 /
CHEB / 1.1744000e-01 6.6926000e-02 4.2669000e-02 /
CHEB / -6.3474000e-02 -2.0470000e-02 -9.3662000e-03 /
CHEB / -8.3927000e-02 -2.3400000e-02 -1.4434000e-02 /

CO+HOC[CH2][CH3]2(+m)=CO2+iC4H9(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #8310 (C5H9O2J(2258))   deltaHrxn(T=298K) = -
25.027086495668335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8496000e+01 -1.7581000e-01 -1.0407000e-01 /
CHEB / 2.3782000e+01 1.7263000e-01 9.9132000e-02 /
CHEB / 1.2736000e+00 3.3722000e-02 2.2398000e-02 /
CHEB / 2.5341000e-01 -1.8278000e-02 -8.8721000e-03 /
CHEB / 1.1886000e-02 -1.2532000e-02 -7.8679000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+H2CCCH3[OH](+m)=CO+HOC[CH2][CH3]2(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #8646 (C5H9O2J(2259))
      deltaHrxn(T=298K) = -19.99825868234338 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5091000e+01 7.1942000e-04 5.0414000e-04 /
CHEB / 2.2496000e+01 -5.7054000e-04 -4.0053000e-04 /
CHEB / 1.5948000e-01 -2.6917000e-04 -1.8756000e-04 /
CHEB / -1.8047000e-03 4.6824000e-05 3.2470000e-05 /
CHEB / -3.6426000e-02 6.5464000e-05 4.5532000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+H2CCCH3[OH](+m)=CO+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9065 (C5H9O2J(2260))
      deltaHrxn(T=298K) = -11.429088529404542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6603000e+01 5.3791000e-08 3.7442000e-08 /
CHEB / 3.2571000e+01 7.7715000e-08 5.4095000e-08 /
CHEB / 4.5794000e-01 4.2558000e-08 2.9623000e-08 /
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CHEB / 1.6062000e-01 2.2728000e-08 1.5820000e-08 /
CHEB / 5.0686000e-02 1.4146000e-08 9.8465000e-09 /

iC4H5OJ(14)+CH3OH(+m)=CH3CO+H2CCCH3[OH](+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9065 (C5H9O2J(2260))
      deltaHrxn(T=298K) = 3.349875676908276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2544000e+00 1.8078000e-07 1.2585000e-07 /
CHEB / 1.5916000e+01 6.9352000e-08 4.8274000e-08 /
CHEB / 3.2600000e-01 -1.0027000e-07 -6.9812000e-08 /
CHEB / 1.3041000e-01 -7.3356000e-08 -5.1068000e-08 /
CHEB / 4.5549000e-02 -1.0698000e-08 -7.4415000e-09 /

iC4H5OJ(14)+CH3OH(+m)=CO+HOC[CH2][CH3]2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #9065 (C5H9O2J(2260))
      deltaHrxn(T=298K) = -8.079212852496266 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3040000e+01 -5.8025000e-06 -4.0390000e-06 /
CHEB / 3.6264000e+01 1.2934000e-06 9.0030000e-07 /
CHEB / 1.2989000e+00 3.5152000e-06 2.4468000e-06 /
CHEB / 4.7402000e-01 1.2976000e-06 9.0322000e-07 /
CHEB / 1.5958000e-01 -1.2422000e-07 -8.6464000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+C2H3(+m)=iC4H7+CH2CHO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9481 (C6H10O(1195))     deltaHrxn(T=298K) = -
46.725237946796454 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2650000e+01 -3.8338000e-01 -1.8449000e-01 /
CHEB / 2.8628000e-02 3.5927000e-01 1.6022000e-01 /
CHEB / 2.3490000e-02 8.0888000e-02 4.5036000e-02 /
CHEB / -3.0189000e-02 -4.4823000e-02 -1.3305000e-02 /
CHEB / -2.3295000e-02 -3.1846000e-02 -1.6828000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     C5H10_iso   -8.56 81.16 26.7  33.51 39.62 44.83 53.13 59.37 69.07
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+sC3H5(+m)=CH3CO+iC4H7(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9941 (C6H10O(2689))     deltaHrxn(T=298K) = -
28.617167044656973 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2898000e+01 -8.3225000e-01 -1.9386000e-01 /
CHEB / -1.1517000e-01 8.1980000e-01 1.3605000e-01 /
CHEB / 3.6567000e-02 1.6238000e-01 8.6846000e-02 /
CHEB / -1.0251000e-01 -8.4651000e-02 7.5589000e-03 /
CHEB / -7.4362000e-02 -7.4769000e-02 -2.7576000e-02 /

CH3CO+iC4H7(+m)=C5H10_iso+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9941 (C6H10O(2689))    deltaHrxn(T=298K) = -
64.99353597180924 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9757000e+00 -5.1838000e-01 -2.0544000e-01 /
CHEB / 1.4566000e+01 5.2573000e-01 1.8776000e-01 /
CHEB / 4.1010000e-01 9.2487000e-02 5.4866000e-02 /
CHEB / 8.5239000e-02 -6.6626000e-02 -1.4732000e-02 /
CHEB / 1.8699000e-02 -4.5678000e-02 -2.3448000e-02 /

CH2C[O]CH3+sC3H5(+m)=C5H10_iso+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9941 (C6H10O(2689))     deltaHrxn(T=298K) = -
93.6107030164662 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0159000e+00 -4.2340000e-01 -1.8080000e-01 /
CHEB / 6.9474000e+00 4.7806000e-01 1.8709000e-01 /
CHEB / 1.0543000e+00 2.1695000e-02 3.0748000e-02 /
CHEB / 2.4248000e-01 -6.6195000e-02 -2.5668000e-02 /
CHEB / 5.0658000e-02 -2.7703000e-02 -1.8580000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(1735)  -31.8 64.6  15.3  17.87 20.17 22.29 25.5  28.18 31.81
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(543)+H(+m)=HO2+CH2CHO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
22.297639095624596 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1464000e+01 -2.2898000e-03 -1.5911000e-03 /
CHEB / -3.4666000e-01 2.3468000e-03 1.6303000e-03 /
CHEB / 1.4449000e-01 3.4225000e-04 2.3813000e-04 /
CHEB / 9.2298000e-02 -3.3741000e-04 -2.3419000e-04 /
CHEB / 3.8773000e-02 -1.4073000e-04 -9.7890000e-05 /

CH2OOH+HCO(+m)=HO2+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
18.687665536037613 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1226000e+01 -4.2630000e-03 -2.9574000e-03 /
CHEB / -2.0686000e-01 4.5630000e-03 3.1641000e-03 /
CHEB / 1.7836000e-01 4.5703000e-04 3.1826000e-04 /
CHEB / 8.2496000e-02 -6.9039000e-04 -4.7806000e-04 /
CHEB / 2.9216000e-02 -2.1388000e-04 -1.4883000e-04 /

nSPC(543)+H(+m)=CH2OOH+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
3.609973559586983 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1206000e+00 -1.9655000e-03 -1.3659000e-03 /
CHEB / 1.1546000e+00 2.1875000e-03 1.5199000e-03 /
CHEB / 5.7172000e-01 6.4810000e-05 4.5457000e-05 /
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CHEB / 1.8015000e-01 -2.8237000e-04 -1.9610000e-04 /
CHEB / 6.6509000e-02 -6.0485000e-05 -4.2188000e-05 /

HO2+CH2CHO(+m)=sSPC(1735)+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
64.93373951207953 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2919000e+00 -3.4329000e-03 -2.3832000e-03 /
CHEB / 7.8748000e+00 3.6194000e-03 2.5117000e-03 /
CHEB / 4.5410000e-01 4.2198000e-04 2.9369000e-04 /
CHEB / 1.4803000e-01 -5.3971000e-04 -3.7409000e-04 /
CHEB / 3.7328000e-02 -1.8729000e-04 -1.3029000e-04 /

nSPC(543)+H(+m)=sSPC(1735)+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
87.23137860770413 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8878000e+00 -1.8872000e-03 -1.3116000e-03 /
CHEB / 2.3623000e+00 2.1236000e-03 1.4755000e-03 /
CHEB / 8.6270000e-01 2.1762000e-05 1.5558000e-05 /
CHEB / 2.7071000e-01 -2.5490000e-04 -1.7705000e-04 /
CHEB / 1.0399000e-01 -5.3761000e-05 -3.7513000e-05 /

CH2OOH+HCO(+m)=sSPC(1735)+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #10491 (C2H4O3(1126))   deltaHrxn(T=298K) = -
83.62140504811714 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9798000e+00 -2.5977000e-03 -1.8041000e-03 /
CHEB / 3.2198000e+00 2.9744000e-03 2.0650000e-03 /
CHEB / 8.2327000e-01 -3.9179000e-05 -2.6236000e-05 /
CHEB / 2.4973000e-01 -3.2572000e-04 -2.2614000e-04 /
CHEB / 9.4369000e-02 -8.3010000e-05 -5.7928000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+CH2CHO(+m)=nSPC(543)+iC4H7(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #10793 (C6H10O3(1671))   deltaHrxn(T=298K) = -
8.00879423925943 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0295000e+01 -4.1491000e-01 -1.7576000e-01 /
CHEB / 1.2677000e+00 4.8960000e-01 1.8969000e-01 /
CHEB / 3.6438000e-01 -5.3176000e-03 2.2373000e-02 /
CHEB / 7.1703000e-03 -6.7019000e-02 -2.7975000e-02 /
CHEB / -2.7042000e-02 -1.7586000e-02 -1.5325000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
```

```
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(97)+CH2CHO(+m)=nSPC(543)+HOC[CH2][CH3]2(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #19 (C6H12O4(450))
      deltaHrxn(T=298K) = 6.229796253196877 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3632000e+00 -5.2249000e-01 -1.8883000e-01 /
CHEB / 4.0292000e+00 6.1329000e-01 1.9327000e-01 /
CHEB / 4.5531000e-01 -5.4210000e-04 3.9692000e-02 /
CHEB / -2.3735000e-02 -8.5946000e-02 -3.1091000e-02 /
CHEB / -7.5839000e-02 -2.5284000e-02 -2.1321000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2C[O]CH3  -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17 41.25
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3CHO            -39.24      62.99 12.97 15.48 17.95 20.18 23.83
      26.59 30.87
!     nSPC(543)   -18.09      77.55 19.79 23.22 26.1  28.39 31.7  33.97
      37.29
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

nSPC(102)+CH3CHO(+m)=CH2C[O]CH3+HO2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C3H6O3JJ(436)) deltaHrxn(T=298K) = -
14.948453876858704 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8524000e+00 -6.9741000e-05 -5.8515000e-05 /
CHEB / 7.1992000e+00 8.0168000e-05 6.6819000e-05 /
CHEB / 2.2169000e-01 2.0161000e-05 1.6800000e-05 /
CHEB / 2.5156000e-02 -3.4460000e-05 -2.8835000e-05 /
CHEB / -3.2545000e-02 -2.9656000e-06 -2.3857000e-06 /
```

```
tSPC(3683)+H(+m)=nSPC(102)+CH3CHO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C3H6O3JJ(436)) deltaHrxn(T=298K) = -
19.057350976908207 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4985000e+00 -9.8834000e-06 -6.9010000e-06 /
CHEB / 5.2812000e+00 6.0853000e-06 4.2663000e-06 /
CHEB / 6.7431000e-01 6.7048000e-06 4.6591000e-06 /
CHEB / 9.0570000e-02 2.0466000e-06 1.4210000e-06 /
CHEB / -3.8638000e-02 -2.4519000e-07 -1.6816000e-07 /

nSPC(543)+CH3(+m)=CH2C[O]CH3+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C3H6O3JJ(436)) deltaHrxn(T=298K) = -
20.237514314041288 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0205000e+00 -2.6239000e-03 -1.8226000e-03 /
CHEB / 6.9410000e+00 3.0418000e-03 2.1126000e-03 /
CHEB / 5.1720000e-01 -4.0983000e-05 -2.8150000e-05 /
CHEB / 1.0684000e-01 -3.7416000e-04 -2.5952000e-04 /
CHEB / 5.0522000e-03 -4.9300000e-05 -3.4552000e-05 /

tSPC(3683)+H(+m)=nSPC(543)+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C3H6O3JJ(436))      deltaHrxn(T=298K) = -
13.76829053972562 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1718000e-01 -6.6282000e-04 -4.6146000e-04 /
CHEB / 6.6095000e+00 7.0534000e-04 4.9104000e-04 /
CHEB / 9.7946000e-01 3.6821000e-05 2.5664000e-05 /
CHEB / 1.6705000e-01 -6.3239000e-05 -4.4047000e-05 /
CHEB / -2.3039000e-02 -2.2799000e-05 -1.5878000e-05 /

nSPC(543)+CH3(+m)=nSPC(102)+CH3CHO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C3H6O3JJ(436)) deltaHrxn(T=298K) = -
5.2890604371825845 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2776000e+00 -5.3077000e-04 -4.4092000e-04 /
CHEB / 3.3673000e+00 6.3369000e-04 5.2611000e-04 /
CHEB / -8.3592000e-02 6.5972000e-05 5.4595000e-05 /
CHEB / -4.8290000e-02 -2.3444000e-04 -1.9445000e-04 /
CHEB / -4.7251000e-02 1.5336000e-05 1.2795000e-05 /

tSPC(3683)+H(+m)=sSPC(1356)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C3H6O3JJ(436))      deltaHrxn(T=298K) = -
9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7350000e+00 -7.6313000e-04 -5.3107000e-04 /
CHEB / 7.4741000e+00 8.1803000e-04 5.6921000e-04 /
CHEB / 1.1702000e+00 3.4497000e-05 2.4098000e-05 /
CHEB / 2.2484000e-01 -7.3549000e-05 -5.1202000e-05 /
CHEB / -3.4946000e-03 -2.4337000e-05 -1.6948000e-05 /
```

```
sSPC(1356)+H(+m)=nSPC(102)+CH3CHO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C3H6O3JJ(436)) deltaHrxn(T=298K) = -
9.438484216720806 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9929000e+00 -6.9762000e-05 -5.8531000e-05 /
CHEB / 3.1746000e+00 8.0149000e-05 6.6806000e-05 /
CHEB / -8.7336000e-02 2.0166000e-05 1.6805000e-05 /
CHEB / -6.0061000e-02 -3.4463000e-05 -2.8838000e-05 /
CHEB / -5.2245000e-02 -2.9775000e-06 -2.3957000e-06 /

sSPC(1356)+H(+m)=nSPC(543)+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C3H6O3JJ(436))      deltaHrxn(T=298K) = -
4.149423779538218 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.4876000e+00 -2.6245000e-03 -1.8231000e-03 /
CHEB / 4.9897000e+00 3.0417000e-03 2.1125000e-03 /
CHEB / 2.9718000e-01 -4.0204000e-05 -2.7609000e-05 /
CHEB / 2.0574000e-02 -3.7378000e-04 -2.5926000e-04 /
CHEB / -2.7735000e-02 -4.9478000e-05 -3.4675000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH3+nSPC(543)(+m)=sSPC(1697)+CH2CHO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #47 (C3H6O3(498))  deltaHrxn(T=298K) = -
4.239556882567771 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8597000e+00 -1.3329000e-02 -9.1640000e-03 /
CHEB / 1.9995000e+00 1.6051000e-02 1.1021000e-02 /
CHEB / 5.9045000e-01 -7.5526000e-04 -5.0336000e-04 /
CHEB / 1.5085000e-01 -2.2374000e-03 -1.5291000e-03 /
CHEB / 4.1707000e-02 -3.7393000e-05 -3.6941000e-05 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     nSPC(543)   -18.09      77.55 19.79 23.22 26.1  28.39 31.7  33.97
      37.29
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:

nSPC(543)+tSPC(346)(+m)=CH2CHO+tSPC(878)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H6O4(410))  deltaHrxn(T=298K)
= -21.67790774292203 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1350000e+00 -1.8237000e-04 -1.2693000e-04 /
CHEB / 2.3901000e+00 8.1970000e-05 5.7049000e-05 /
CHEB / 7.9489000e-01 -1.2205000e-05 -8.4943000e-06 /
CHEB / 2.0088000e-01 -5.2866000e-05 -3.6793000e-05 /
CHEB / 1.8352000e-02 -2.6555000e-05 -1.8482000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
nSPC(543)+C3H3O-enone(+m)=tSPC(1286)+CH2CHO(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #225 (C5H6O4(761))
      deltaHrxn(T=298K) = 0.879793215632362 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4208000e+00 -9.8605000e-02 -6.2605000e-02 /
CHEB / 4.0692000e+00 9.6021000e-02 5.9370000e-02 /
CHEB / 8.0412000e-01 1.7076000e-03 1.8759000e-03 /
CHEB / 1.5832000e-01 -1.6739000e-02 -1.0337000e-02 /
CHEB / 2.0490000e-02 -4.1372000e-03 -2.9429000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C2H4O=CH3CH[OH]CH2  1.3600000e+12      0.00000
1.0100000e+04
!     C3H6+OH=CH3CH[OH]CH2    2.7100000e+12      0.00000
0.0000000e+00
!     H2CCCH3[OH]+H=CH3CH[OH]CH2    1.1700000e+13      0.00000
4.7000000e+03
!     CH3CH[OH]CH2=CH3C[OH]CH3      6.2339791e+09      0.93630
3.7689907e+04

CH3+C2H4O(+m)=CH3CH[OH]CH2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2) High-P Limit: R_Addition_MultipleBond
exact:  C_methyl     Cd/H/Nd_Cd/H2        deltaHrxn(T=298K) = -
21.697420406016636 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8498000e+00 1.1873000e+00 -2.0872000e-01 /
CHEB / 4.3710000e-01 9.0293000e-01 1.3271000e-01 /
CHEB / -1.9179000e+00 2.8839000e-01 6.1292000e-02 /
CHEB / -9.8303000e-01 -3.2509000e-02 1.1881000e-02 /
CHEB / -4.5763000e-01 -8.5272000e-02 -1.1086000e-02 /
```

```
C3H6+OH(+m)=CH3CH[OH]CH2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     O_pri_rad      deltaHrxn(T=298K)
= -30.466609425124325 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0878000e+01 8.5602000e-01 -1.0083000e-01 /
CHEB / -3.1158000e+00 9.2979000e-01 5.0826000e-02 /
CHEB / -1.8848000e+00 2.9888000e-01 5.5526000e-02 /
CHEB / -1.0111000e+00 -2.5149000e-02 2.0003000e-02 /
CHEB / -4.8519000e-01 -8.3936000e-02 -8.2399000e-03 /

H2CCCH3[OH]+H(+m)=CH3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2)     deltaHrxn(T=298K) = -
4.9893206475953455 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0658000e+01 -6.1737000e-01 -1.4954000e-01 /
CHEB / 2.0145000e+00 7.4896000e-01 1.4279000e-01 /
CHEB / 1.2356000e-02 -4.7580000e-02 4.2993000e-02 /
CHEB / -2.7030000e-02 -8.3435000e-02 -2.1290000e-02 /
CHEB / 2.3504000e-02 -1.4562000e-02 -1.9515000e-02 /

H2CCCH3[OH]+H(+m)=C3H6+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2)     deltaHrxn(T=298K) =
3.7798683715123422 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1112000e+01 -6.6260000e-01 -1.5584000e-01 /
CHEB / 1.6523000e+00 7.7722000e-01 1.4586000e-01 /
CHEB / -5.7509000e-02 -9.6674000e-03 4.5740000e-02 /
CHEB / -3.3257000e-02 -9.7335000e-02 -1.7998000e-02 /
CHEB / 2.1449000e-02 -2.4771000e-02 -2.0156000e-02 /

H2CCCH3[OH]+H(+m)=CH3C[OH]CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2)     deltaHrxn(T=298K) = -
33.28625839425898 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1124000e+00 -3.8984000e-01 -1.6504000e-01 /
CHEB / 4.1165000e+00 4.7013000e-01 1.8597000e-01 /
CHEB / 3.0712000e-01 -1.9607000e-02 8.8831000e-03 /
CHEB / 1.0228000e-01 -6.3840000e-02 -2.4948000e-02 /
CHEB / 6.2645000e-02 -8.7751000e-03 -9.9099000e-03 /

CH3+C2H4O(+m)=CH3C[OH]CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2)     deltaHrxn(T=298K) = -
28.296937746663637 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3285000e+00 -3.8984000e-01 -1.6504000e-01 /
CHEB / 6.4503000e+00 4.7013000e-01 1.8597000e-01 /
CHEB / 3.0203000e-01 -1.9607000e-02 8.8831000e-03 /
CHEB / 9.2017000e-02 -6.3840000e-02 -2.4948000e-02 /
CHEB / 5.6484000e-02 -8.7751000e-03 -9.9099000e-03 /
```

```
C3H6+OH(+m)=CH3C[OH]CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #299 (CH3CH[OH]CH2)     deltaHrxn(T=298K) = -
37.06612676577133 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6770000e+00 -4.0483000e-01 -1.7348000e-01 /
CHEB / 3.2090000e+00 4.7847000e-01 1.9244000e-01 /
CHEB / 2.1476000e-01 -4.4534000e-03 1.3437000e-02 /
CHEB / 4.6205000e-02 -6.9778000e-02 -2.6033000e-02 /
CHEB / 2.8371000e-02 -1.3045000e-02 -1.1349000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C8H14       3.28  104.5 41.02 51.34 60.44 68.08 80.22 89.2  102.98
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+iC4H7(+m)=C8H14+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #317 (C8H15O2J(1448))   deltaHrxn(T=298K) = -
6.529179555716089 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5971000e+00 -6.3690000e-01 -1.7426000e-01 /
CHEB / 4.6699000e+00 7.8865000e-01 1.7235000e-01 /
CHEB / -4.1567000e-01 -4.0664000e-02 6.1660000e-02 /
CHEB / -3.0008000e-01 -1.1985000e-01 -4.6115000e-02 /
CHEB / -1.6395000e-01 -3.2211000e-02 -3.4110000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C8H14       3.28  104.5 41.02 51.34 60.44 68.08 80.22 89.2  102.98
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
```

```
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

C8H14+O(+m)=C4H7OJ(79)+iC4H7(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #463 (C8H14OJJ(1626))   deltaHrxn(T=298K) = -
16.828133060700843 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0876000e+00 -2.3124000e-03 -1.6067000e-03 /
CHEB / 3.7026000e+00 2.9349000e-03 2.0385000e-03 /
CHEB / 5.5712000e-01 -4.3685000e-04 -3.0238000e-04 /
CHEB / 7.3966000e-02 -2.2198000e-04 -1.5459000e-04 /
CHEB / -3.3319000e-02 3.8026000e-06 2.5060000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+tSPC(1553)(+m)=CH2C[O]CH3+C3H3O-enone(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #587 (C6H8O2(1937))
      deltaHrxn(T=298K) = -26.157610672260695 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2805000e+01 -4.0783000e-01 -1.7548000e-01 /
CHEB / 8.7827000e-02 4.7899000e-01 1.9062000e-01 /
CHEB / 1.6943000e-02 -3.5956000e-03 1.6324000e-02 /
CHEB / -1.7467000e-02 -6.4231000e-02 -2.0236000e-02 /
CHEB / 1.0194000e-02 -1.4421000e-02 -1.5560000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+sSPC(1590)(+m)=tSPC(1553)+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1328 (C6H8O3JJ(2221))
      deltaHrxn(T=298K) = -8.509389394409972 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0229000e+01 -6.9117000e-01 2.0150000e-01 /
CHEB / 1.6943000e+00 4.4190000e-01 -2.1039000e-01 /
CHEB / 1.7764000e-01 2.4107000e-01 -6.7090000e-02 /
CHEB / -1.5607000e-01 1.5949000e-01 3.4232000e-02 /
CHEB / -8.9228000e-02 -2.0013000e-02 5.3805000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+tSPC(1286)(+m)=CH2C[O]CH3+tSPC(1553)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1913 (C6H8O3(2094))
      deltaHrxn(T=298K) = -77.36208657838935 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3276000e+01 3.7010000e-09 2.5762000e-09 /
CHEB / -5.2280000e-01 7.2502000e-09 5.0466000e-09 /
CHEB / -2.8833000e-02 6.8036000e-09 4.7358000e-09 /
CHEB / -1.5971000e-03 6.0884000e-09 4.2380000e-09 /
CHEB / -7.2119000e-03 5.1432000e-09 3.5801000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+C4H7OJ(79)(+m)=CH2C[O]CH3+iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2172 (C7H12O(1938))     deltaHrxn(T=298K) = -
45.855343398031124 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2525000e+01 -5.9985000e-01 -2.3443000e-01 /
CHEB / 1.5885000e-01 5.8256000e-01 2.0044000e-01 /
CHEB / 5.4207000e-02 1.4082000e-01 7.7478000e-02 /
CHEB / -5.4152000e-02 -6.4183000e-02 -5.1064000e-03 /
CHEB / -4.6085000e-02 -6.1003000e-02 -2.8202000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3O             4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+CH3O(+m)=CH2C[O]CH3+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3140 (C4H8O(1933))     deltaHrxn(T=298K) = -
33.817006388397054 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2792000e+01 -2.7752000e-01 -1.4989000e-01 /
CHEB / -1.1688000e-01 2.3575000e-01 1.2396000e-01 /
CHEB / 2.7192000e-02 8.8317000e-02 4.6907000e-02 /
CHEB / -1.3266000e-02 -1.9292000e-02 -5.4417000e-03 /
CHEB / -1.9163000e-02 -2.3812000e-02 -1.1969000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     acetone     -51.56      70.09 17.97 22.0  25.89 29.34 34.93 39.15
      44.77 null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     CH2C[OH]CH2 -2.71 70.86 18.56 22.7  25.99 28.7  33.11 36.26 40.88
      null
!Here are the path reactions and their high-P limit kinetics:

H2CCCH3[OH]+CH2(+m)=acetone+CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
12.748562463513409 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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```
CHEB / 5    3 /
CHEB / 1.9299000e+00 -1.5429000e-03 -1.0729000e-03 /
CHEB / 7.6458000e+00 1.8793000e-03 1.3065000e-03 /
CHEB / 9.1720000e-01 -1.6744000e-04 -1.1610000e-04 /
CHEB / 2.6381000e-01 -1.8852000e-04 -1.3110000e-04 /
CHEB / 8.2229000e-02 2.6548000e-06 1.7444000e-06 /

O+iC4H8(+m)=H2CCCH3[OH]+CH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
2.219928328647754 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5710000e-01 -1.4722000e-03 -1.0239000e-03 /
CHEB / 8.4638000e+00 1.8209000e-03 1.2662000e-03 /
CHEB / 1.1962000e+00 -2.2118000e-04 -1.5352000e-04 /
CHEB / 2.8358000e-01 -1.3904000e-04 -9.6777000e-05 /
CHEB / 7.0546000e-02 -5.6927000e-06 -4.0189000e-06 /

H2CCCH3[OH]+CH2(+m)=CH2C[O]CH3+CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3357 (C4H8OJJ(480))     deltaHrxn(T=298K) = -
21.62779213848721 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9570000e-01 -1.5429000e-03 -1.0729000e-03 /
CHEB / 7.4696000e+00 1.8793000e-03 1.3065000e-03 /
CHEB / 8.7089000e-01 -1.6744000e-04 -1.1610000e-04 /
CHEB / 2.4759000e-01 -1.8852000e-04 -1.3110000e-04 /
CHEB / 7.5843000e-02 2.6548000e-06 1.7444000e-06 /

acetone+CH2(+m)=OH+iC4H7(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) =
0.8397055715610762 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5575000e-01 -5.4650000e-04 -3.8084000e-04 /
CHEB / 1.0931000e+01 5.8305000e-04 4.0645000e-04 /
CHEB / 5.9529000e-01 6.5964000e-05 4.5764000e-05 /
CHEB / 2.0705000e-01 -9.3803000e-05 -6.5339000e-05 /
CHEB / 6.6226000e-02 -1.9512000e-05 -1.3559000e-05 /

O+iC4H8(+m)=OH+iC4H7(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
14.12878522060008 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4820000e+00 -6.5201000e-04 -4.5420000e-04 /
CHEB / 7.3582000e+00 7.4165000e-04 5.1676000e-04 /
CHEB / 9.3956000e-01 8.6745000e-06 5.8726000e-06 /
CHEB / 2.4150000e-01 -1.0034000e-04 -6.9854000e-05 /
CHEB / 6.4466000e-02 -6.0453000e-06 -4.1912000e-06 /

OH+iC4H7(+m)=CH2C[O]CH3+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
9.718935246534876 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2258000e+00 -5.4650000e-04 -3.8084000e-04 /
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CHEB / 1.0140000e+01 5.8305000e-04 4.0645000e-04 /
CHEB / 3.8503000e-01 6.5964000e-05 4.5764000e-05 /
CHEB / 1.2727000e-01 -9.3803000e-05 -6.5339000e-05 /
CHEB / 3.1065000e-02 -1.9512000e-05 -1.3559000e-05 /

H2CCCH3[OH]+CH2(+m)=OH+iC4H7(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
11.908856891952333 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0909000e+00 -1.3047000e-03 -9.0828000e-04 /
CHEB / 2.2158000e+00 1.5908000e-03 1.1075000e-03 /
CHEB / 2.2913000e-01 -1.3615000e-04 -9.4861000e-05 /
CHEB / 7.9078000e-02 -1.5806000e-04 -1.0998000e-04 /
CHEB / 2.1706000e-02 -1.2133000e-05 -8.4671000e-06 /

acetone+CH2(+m)=CH2C[OH]CH2+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
8.679300087961273 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0661000e-01 -5.4650000e-04 -3.8084000e-04 /
CHEB / 1.0586000e+01 5.8305000e-04 4.0645000e-04 /
CHEB / 5.0460000e-01 6.5964000e-05 4.5764000e-05 /
CHEB / 1.7528000e-01 -9.3803000e-05 -6.5339000e-05 /
CHEB / 5.3722000e-02 -1.9512000e-05 -1.3559000e-05 /

O+iC4H8(+m)=CH2C[OH]CH2+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
23.64779088012243 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2443000e+00 -6.5201000e-04 -4.5420000e-04 /
CHEB / 7.0131000e+00 7.4165000e-04 5.1676000e-04 /
CHEB / 8.4888000e-01 8.6745000e-06 5.8726000e-06 /
CHEB / 2.0973000e-01 -1.0034000e-04 -6.9854000e-05 /
CHEB / 5.1962000e-02 -6.0453000e-06 -4.1912000e-06 /

CH2C[O]CH3+CH3(+m)=CH2C[OH]CH2+CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3357 (C4H8OJJ(480))     deltaHrxn(T=298K) =
0.1999295870125266 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2388000e+00 -5.4650000e-04 -3.8084000e-04 /
CHEB / 1.3415000e+01 5.8305000e-04 4.0645000e-04 /
CHEB / 4.6410000e-01 6.5964000e-05 4.5764000e-05 /
CHEB / 1.6665000e-01 -9.3803000e-05 -6.5339000e-05 /
CHEB / 4.8107000e-02 -1.9512000e-05 -1.3559000e-05 /

H2CCCH3[OH]+CH2(+m)=CH2C[OH]CH2+CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3357 (C4H8OJJ(480))     deltaHrxn(T=298K) = -
21.427862551474682 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8533000e+00 -1.3047000e-03 -9.0828000e-04 /
CHEB / 1.8708000e+00 1.5908000e-03 1.1075000e-03 /
CHEB / 1.3845000e-01 -1.3615000e-04 -9.4861000e-05 /
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CHEB / 4.7310000e-02 -1.5806000e-04 -1.0998000e-04 /
CHEB / 9.2017000e-03 -1.2133000e-05 -8.4671000e-06 /

OH+iC4H7(+m)=CH2C[OH]CH2+CH3(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3357 (C4H8OJJ(480))    deltaHrxn(T=298K) = -
9.51900565952235 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0988000e+01 -3.2934000e-03 -2.2858000e-03 /
CHEB / 1.1721000e+00 4.3076000e-03 2.9883000e-03 /
CHEB / 1.0990000e-01 -7.8591000e-04 -5.4297000e-04 /
CHEB / -3.4921000e-02 -2.9532000e-04 -2.0594000e-04 /
CHEB / -3.1573000e-02 1.7275000e-05 1.1758000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+C2H3(+m)=sC3H5+CH2CHO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3667 (C5H8O(2084))      deltaHrxn(T=298K) = -
0.8698945487653331 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0045000e+01 -1.3717000e+00 -5.8782000e-02 /
CHEB / 2.5055000e+00 9.9042000e-01 -5.3119000e-02 /
CHEB / 1.9400000e-01 4.6338000e-01 3.9457000e-02 /
CHEB / -1.8529000e-01 6.5745000e-02 5.9170000e-02 /
CHEB / -1.4122000e-01 -8.3211000e-02 2.4591000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
```

```
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     CH2C[O]CH3  -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17 41.25
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

iC4H7+sSPC(1356)(+m)=tSPC(54)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O3JJ(391))
      deltaHrxn(T=298K) = 3.4794910670479338 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7963000e+00 -1.1457000e-01 -7.1571000e-02 /
CHEB / 1.7831000e+01 1.3805000e-01 8.4785000e-02 /
CHEB / -1.0886000e-01 -3.3419000e-03 1.6763000e-04 /
CHEB / -1.2448000e-01 -2.1129000e-02 -1.3455000e-02 /
CHEB / -5.8548000e-02 -4.8244000e-03 -3.7526000e-03 /

iC4H7+sSPC(1356)(+m)=tSPC(77)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O3JJ(391))
      deltaHrxn(T=298K) = 3.479317234229476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8499000e+01 -7.6958000e-02 -4.9894000e-02 /
CHEB / 2.2824000e+01 1.0190000e-01 6.5343000e-02 /
CHEB / 5.6995000e-01 -1.6289000e-02 -9.2460000e-03 /
CHEB / 5.4092000e-02 -1.3034000e-02 -8.9231000e-03 /
CHEB / -2.2122000e-02 1.8369000e-03 8.7348000e-04 /

tSPC(54)+CH2C[O]CH3(+m)=tSPC(77)+CH2C[O]CH3(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O3JJ(391))
      deltaHrxn(T=298K) = -1.7383281845795295E-4 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7971000e+01 -7.7285000e-02 -4.9927000e-02 /
CHEB / 2.2143000e+01 1.0255000e-01 6.5531000e-02 /
CHEB / 6.3305000e-01 -1.6862000e-02 -9.5887000e-03 /
CHEB / 7.3024000e-02 -1.2796000e-02 -8.7436000e-03 /
CHEB / -2.4008000e-02 1.9467000e-03 9.5941000e-04 /
```

```
tSPC(3683)+iC4H7(+m)=iC4H7+sSPC(1356)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C7H12O3JJ(391))      deltaHrxn(T=298K) = -
9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6303000e+01 -7.0486000e-02 -4.6015000e-02 /
CHEB / 1.9804000e+01 9.4602000e-02 6.1137000e-02 /
CHEB / 5.0944000e-01 -1.7140000e-02 -1.0031000e-02 /
CHEB / 3.0827000e-02 -1.1265000e-02 -7.8195000e-03 /
CHEB / -3.2812000e-02 2.2520000e-03 1.2236000e-03 /

tSPC(3683)+iC4H7(+m)=tSPC(54)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O3JJ(391))
      deltaHrxn(T=298K) = -6.139375693139468 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6051000e+01 -7.1271000e-02 -4.6329000e-02 /
CHEB / 2.0237000e+01 9.5782000e-02 6.1638000e-02 /
CHEB / 5.5197000e-01 -1.7700000e-02 -1.0348000e-02 /
CHEB / 4.5244000e-02 -1.1106000e-02 -7.6844000e-03 /
CHEB / -3.1092000e-02 2.3546000e-03 1.2887000e-03 /

tSPC(3683)+iC4H7(+m)=tSPC(77)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O3JJ(391))
      deltaHrxn(T=298K) = -6.139549525957926 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9328000e+00 -1.4603000e-03 -1.0152000e-03 /
CHEB / 1.6510000e+01 1.9078000e-03 1.3260000e-03 /
CHEB / 2.4769000e-01 -3.5176000e-04 -2.4404000e-04 /
CHEB / 3.5543000e-03 -1.2052000e-04 -8.3987000e-05 /
CHEB / -8.1611000e-02 7.5476000e-06 5.2022000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

iC4H7+sSPC(1356)(+m)=C4H7OJ(79)+sSPC(1590)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4962 (C7H12O3(1380))
      deltaHrxn(T=298K) = -18.938011541560726 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2714000e+01 -6.6627000e-01 -1.8514000e-01 /
CHEB / 1.1339000e-01 7.6563000e-01 1.7201000e-01 /
CHEB / -4.1297000e-02 2.8574000e-02 6.2620000e-02 /
CHEB / -8.6959000e-02 -1.1393000e-01 -2.6846000e-02 /
CHEB / -3.0005000e-02 -4.5598000e-02 -3.0921000e-02 /

tSPC(54)+CH2C[O]CH3(+m)=C4H7OJ(79)+sSPC(1590)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4962 (C7H12O3(1380))
      deltaHrxn(T=298K) = -30.12635480957534 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2884000e+01 -2.8415000e-01 -1.5405000e-01 /
CHEB / -1.5486000e-01 3.3155000e-01 1.7248000e-01 /
CHEB / -4.3665000e-02 9.8370000e-03 1.4643000e-02 /
CHEB / -3.9129000e-02 -5.6153000e-02 -2.8296000e-02 /
CHEB / -2.5543000e-02 -1.6852000e-02 -1.3425000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+tSPC(122)(+m)=sSPC(1356)+tSPC(77)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O5(487)) deltaHrxn(T=298K)
= -11.188343229150071 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1749000e+00 -3.3864000e-01 -1.5510000e-01 /
CHEB / 2.3253000e+00 4.2211000e-01 1.8174000e-01 /
CHEB / 4.0647000e-01 -2.9368000e-02 4.7678000e-03 /
CHEB / 2.0734000e-03 -6.4080000e-02 -3.1648000e-02 /
CHEB / -4.1456000e-02 -6.1520000e-03 -8.9273000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+tSPC(3683)(+m)=sSPC(1356)+tSPC(77)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O5JJ(404))
      deltaHrxn(T=298K) = -9.61904059300586 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0983000e+00 -5.3355000e-01 -1.8772000e-01 /
CHEB / 1.6548000e+01 6.6121000e-01 2.0375000e-01 /
CHEB / -8.4206000e-02 -3.5180000e-02 3.4642000e-02 /
CHEB / -1.3459000e-01 -1.0751000e-01 -4.5343000e-02 /
CHEB / -4.8825000e-02 -1.5602000e-02 -2.1667000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(122)+CH2CHO(+m)=nSPC(543)+tSPC(77)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #25 (C6H10O5(357))
      deltaHrxn(T=298K) = -8.008794200394888 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6722000e+00 -6.0479000e-01 -1.7796000e-01 /
CHEB / 1.2546000e+00 7.3449000e-01 1.8016000e-01 /
CHEB / 2.0264000e-01 -2.7662000e-02 4.7027000e-02 /
CHEB / -4.5779000e-02 -1.0797000e-01 -3.7832000e-02 /
CHEB / -3.7638000e-02 -2.3542000e-02 -2.3822000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(97)+CH2C[O]CH3(+m)=sSPC(1356)+HOC[CH2][CH3]2(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #43 (C7H14O4(576))
      deltaHrxn(T=298K) = 3.0502472244416943 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7546000e+00 -3.8499000e-01 -1.6557000e-01 /
CHEB / 4.8426000e+00 4.7374000e-01 1.8837000e-01 /
CHEB / 7.6204000e-01 -2.6019000e-02 1.2331000e-02 /
CHEB / 5.8567000e-02 -7.1030000e-02 -3.2718000e-02 /
CHEB / -4.3229000e-02 -9.3715000e-03 -1.2046000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
```

```
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+sSPC(1356)(+m)=tSPC(1553)+sSPC(1590)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #136 (C6H8O4JJ(1019))
      deltaHrxn(T=298K) = -38.635744267331134 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2663000e+01 -1.0248000e-02 -8.5024000e-03 /
CHEB / 8.9380000e-02 1.0105000e-02 8.4223000e-03 /
CHEB / 5.6929000e-03 3.9083000e-03 3.1651000e-03 /
CHEB / 2.0887000e-02 -3.6190000e-03 -2.9674000e-03 /
CHEB / 3.6552000e-03 -1.1438000e-03 -9.2461000e-04 /

C3H3O-enone+sSPC(1356)(+m)=tSPC(1286)+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #136 (C6H8O4JJ(1019))
      deltaHrxn(T=298K) = 4.059342244387543 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8242000e+00 -1.4879000e-02 -1.0207000e-02 /
CHEB / 5.7524000e+00 1.6425000e-02 1.1247000e-02 /
CHEB / 1.0015000e+00 1.4121000e-03 9.8701000e-04 /
CHEB / 2.1393000e-01 -2.8763000e-03 -1.9579000e-03 /
CHEB / 1.2603000e-02 -6.5800000e-04 -4.6132000e-04 /

tSPC(1286)+CH2C[O]CH3(+m)=tSPC(1553)+sSPC(1590)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #136 (C6H8O4JJ(1019))
      deltaHrxn(T=298K) = -42.695086511718685 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2780000e+01 -3.6016000e-03 -3.0309000e-03 /
CHEB / -1.3416000e-01 3.0852000e-03 2.6043000e-03 /
CHEB / -4.9780000e-02 2.1278000e-03 1.7761000e-03 /
CHEB / -9.5117000e-03 -1.3726000e-03 -1.1530000e-03 /
CHEB / -2.1217000e-02 -6.8726000e-04 -5.7051000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+CH2C[O]CH3(+m)=tSPC(346)+sSPC(1356)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #236 (C6H8O4(698))
      deltaHrxn(T=298K) = -3.9991069075749124 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2896000e+00 -2.8168000e-05 -1.9607000e-05 /
CHEB / 4.1689000e+00 2.4091000e-05 1.6769000e-05 /
CHEB / 1.1236000e+00 7.6674000e-06 5.3370000e-06 /
CHEB / 2.6772000e-01 -2.5553000e-06 -1.7786000e-06 /
CHEB / 3.6813000e-02 -1.7233000e-06 -1.1995000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     sSPC(2810)  -29.51      59.94 9.81  11.32 12.68 13.78 15.39 16.47
      17.98
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+sSPC(2810)(+m)=sSPC(1356)+CH2CHO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -10.56897678524659 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -1.0355000e+01 -1.4826000e-06 -1.0320000e-06 /
CHEB / 1.7281000e+01 -3.8194000e-07 -2.6586000e-07 /
CHEB / 4.4459000e-01 1.3793000e-06 9.6011000e-07 /
CHEB / 1.3353000e-01 7.7666000e-07 5.4062000e-07 /
CHEB / -2.4744000e-02 -5.1143000e-08 -3.5599000e-08 /

tSPC(54)+sSPC(2810)(+m)=tSPC(77)+sSPC(2810)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -1.7383281845795295E-4 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8585000e+01 -3.2216000e-06 -2.2425000e-06 /
CHEB / 2.1807000e+01 -7.3520000e-07 -5.1175000e-07 /
CHEB / 1.0026000e+00 2.9309000e-06 2.0401000e-06 /
CHEB / 2.2801000e-01 1.5712000e-06 1.0936000e-06 /
CHEB / -3.7110000e-02 -7.7992000e-08 -5.4288000e-08 /

tSPC(77)+sSPC(2810)(+m)=sSPC(1356)+CH2CHO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -10.568802952428133 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5700000e+01 -2.8239000e-06 -1.9657000e-06 /
CHEB / 1.9901000e+01 -6.7025000e-07 -4.6655000e-07 /
CHEB / 7.4520000e-01 2.6377000e-06 1.8361000e-06 /
CHEB / 1.7715000e-01 1.4071000e-06 9.7943000e-07 /
CHEB / -3.4203000e-02 -1.1637000e-07 -8.1001000e-08 /

tSPC(54)+sSPC(2810)(+m)=tSPC(3683)+CH2CHO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -0.9501100250591881 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7640000e+01 -3.2216000e-06 -2.2425000e-06 /
CHEB / 2.1487000e+01 -7.3520000e-07 -5.1175000e-07 /
CHEB / 9.1843000e-01 2.9309000e-06 2.0401000e-06 /
CHEB / 1.9854000e-01 1.5712000e-06 1.0936000e-06 /
CHEB / -4.8710000e-02 -7.7992000e-08 -5.4288000e-08 /

tSPC(3683)+CH2CHO(+m)=sSPC(1356)+CH2CHO(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5888000e+01 -2.8239000e-06 -1.9657000e-06 /
CHEB / 2.0055000e+01 -6.7025000e-07 -4.6655000e-07 /
CHEB / 7.4214000e-01 2.6377000e-06 1.8361000e-06 /
CHEB / 1.7794000e-01 1.4071000e-06 9.7943000e-07 /
CHEB / -3.6467000e-02 -1.1637000e-07 -8.1001000e-08 /

tSPC(77)+sSPC(2810)(+m)=tSPC(3683)+CH2CHO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C5H8O4JJ(349))
      deltaHrxn(T=298K) = -0.9499361922407301 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2345000e+01 -1.4803000e-06 -1.0304000e-06 /
```

```
CHEB / 1.8759000e+01 -2.4319000e-07 -1.6927000e-07 /
CHEB / 4.5595000e-01 1.3695000e-06 9.5329000e-07 /
CHEB / 1.5123000e-02 6.4495000e-07 4.4893000e-07 /
CHEB / -2.8176000e-02 -9.9713000e-08 -6.9407000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+nSPC(543)(+m)=sSPC(1356)+CH2CHO(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #582 (C5H8O4(489))
      deltaHrxn(T=298K) = -3.179549028755182 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1435000e+00 -1.9028000e-01 -1.0709000e-01 /
CHEB / 2.5607000e+00 2.2053000e-01 1.1950000e-01 /
CHEB / 5.4622000e-01 -5.9635000e-03 1.8869000e-03 /
CHEB / 7.7989000e-02 -3.0962000e-02 -1.7227000e-02 /
CHEB / -6.2787000e-03 -5.8501000e-03 -4.9740000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
```

```
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+CH2C[O]CH3(+m)=iC4H7+sSPC(2810)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #832 (C5H8O2JJ(507))
      deltaHrxn(T=298K) = -9.37906339209242 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0813000e+00 -1.2033000e-06 -8.3758000e-07 /
CHEB / 1.6067000e+01 -1.6870000e-07 -1.1743000e-07 /
CHEB / 2.3745000e-01 1.1657000e-06 8.1140000e-07 /
CHEB / 3.3795000e-02 5.1900000e-07 3.6126000e-07 /
CHEB / 2.4397000e-03 -1.2410000e-07 -8.6385000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     CH2C[O]CH3  -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17 41.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

sC3H5+O2(+m)=aC3H4+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (blah1)  deltaHrxn(T=298K) = -12.458720408841181 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1917000e+01 -3.2948000e-02 -3.0493000e-02 /
CHEB / 2.9062000e-01 4.2642000e-02 3.8663000e-02 /
CHEB / 7.8705000e-02 -3.3798000e-03 -2.4155000e-03 /
CHEB / 2.4061000e-02 -8.8104000e-03 -7.4889000e-03 /
CHEB / 9.2077000e-03 2.3620000e-04 -1.9101000e-04 /
```

```
sC3H5+O2(+m)=CH2C[O]CH3+O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (blah1)  deltaHrxn(T=298K) = -9.149150060377941 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3087000e+01 -4.9945000e-02 -3.6617000e-02 /
CHEB / -5.2042000e-01 6.2756000e-02 4.5919000e-02 /
CHEB / -8.8915000e-02 -4.7831000e-03 -3.4530000e-03 /
CHEB / -4.9453000e-02 -1.0312000e-02 -7.3796000e-03 /
CHEB / -2.7734000e-02 1.8410000e-04 -1.9005000e-05 /

CH2C[O]CH3+O(+m)=aC3H4+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (blah1)  deltaHrxn(T=298K) = -3.3095703484632324 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2860000e+01 -6.4810000e-01 -1.4321000e-01 /
CHEB / -7.7463000e-02 7.7828000e-01 1.3918000e-01 /
CHEB / 3.3060000e-03 -2.4908000e-02 3.8526000e-02 /
CHEB / -1.4058000e-02 -1.0651000e-01 -2.0004000e-02 /
CHEB / 1.8182000e-02 -2.2667000e-02 -1.9474000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+sSPC(2810)(+m)=CH2CHO+sSPC(1590)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1081 (C5H8O3JJ(1257))
      deltaHrxn(T=298K) = -1.8092799392680199 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1405000e+01 -2.0226000e-06 -1.4079000e-06 /
CHEB / 1.8419000e+01 -2.5368000e-07 -1.7658000e-07 /
CHEB / 3.7072000e-01 1.9329000e-06 1.3455000e-06 /
CHEB / 5.4913000e-02 8.5907000e-07 5.9797000e-07 /
CHEB / 3.2935000e-02 -1.8254000e-07 -1.2706000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+C2H3(+m)=sSPC(1590)+CH2CHO(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1168 (C5H8O3(1244))     deltaHrxn(T=298K) = -
65.66324948835717 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3525000e+01 -4.9363000e-05 -3.4358000e-05 /
CHEB / -7.2336000e-01 -5.6154000e-05 -3.9083000e-05 /
CHEB / -2.7223000e-02 -4.2774000e-05 -2.9771000e-05 /
CHEB / 1.3692000e-03 -3.5624000e-05 -2.4794000e-05 /
CHEB / -5.5337000e-03 -2.3368000e-05 -1.6264000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     acetone     -51.21      70.9  17.53 21.65 25.52 28.9  34.34 38.41
      44.77
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
```

```
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2              93.85 46.59 8.3   8.66  8.98  9.28  9.87  10.47
      11.69
!     sSPC(1474)  -67.94      85.82 28.37 33.77 38.22 41.77 46.97 50.61
      56.09
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     CH2C[O]CH3  -6.15 72.93 17.86 21.85 25.33 28.26 32.82 36.17 41.25
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2              3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!Here are the path reactions and their high-P limit kinetics:

CH3+sSPC(1356)(+m)=acetone+nSPC(102)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
4.558982197234791 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3570000e+00 -3.0929000e-04 -2.5127000e-04 /
CHEB / 3.2639000e+00 3.9952000e-04 3.2424000e-04 /
CHEB / -1.0788000e-01 -2.3733000e-05 -1.8742000e-05 /
CHEB / -6.8480000e-02 -1.1132000e-04 -9.0763000e-05 /
CHEB / -6.4386000e-02 3.4153000e-05 2.7815000e-05 /

C4H8O2(62)+O(+m)=CH3+sSPC(1356)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O3JJ(334))      deltaHrxn(T=298K) = -
33.116646192761735 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1768000e+00 -1.4201000e-04 -9.8943000e-05 /
CHEB / 2.1345000e+00 1.2410000e-04 8.6499000e-05 /
CHEB / 2.6921000e-01 4.4984000e-05 3.1295000e-05 /
CHEB / 6.6106000e-03 -1.7204000e-05 -1.1995000e-05 /
CHEB / -5.0878000e-02 -7.9897000e-06 -5.5544000e-06 /

C4H8O2(62)+O(+m)=acetone+nSPC(102)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
37.675628389996525 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3716000e+00 1.1981000e-04 8.3420000e-05 /
CHEB / 1.0777000e+00 -1.5366000e-04 -1.0701000e-04 /
CHEB / -7.6530000e-02 2.3847000e-05 1.6627000e-05 /
CHEB / -1.0349000e-01 1.4697000e-05 1.0222000e-05 /
CHEB / -8.5874000e-02 -2.2735000e-06 -1.5838000e-06 /

CH2+sSPC(1474)(+m)=CH3+sSPC(1356)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
21.447555705883335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2708000e+00 -8.7544000e-04 -6.1004000e-04 /
CHEB / 2.9185000e+00 1.1023000e-03 7.6830000e-04 /
CHEB / 3.1911000e-01 -1.4993000e-04 -1.0477000e-04 /
CHEB / 5.8023000e-02 -9.7486000e-05 -6.7804000e-05 /
```

```
CHEB / -1.3344000e-02 2.1293000e-05 1.4829000e-05 /

CH2+sSPC(1474)(+m)=acetone+nSPC(102)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
26.006537903118122 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7145000e+00 -4.8149000e-05 -3.4806000e-05 /
CHEB / 1.6661000e+00 7.1949000e-05 5.2041000e-05 /
CHEB / -5.9175000e-02 -1.1136000e-05 -8.5106000e-06 /
CHEB / -5.2462000e-02 -3.0594000e-05 -2.1281000e-05 /
CHEB / -4.6908000e-02 2.1309000e-05 1.4938000e-05 /

C4H8O2(62)+O(+m)=CH2+sSPC(1474)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O3JJ(334))      deltaHrxn(T=298K) = -
11.669090486878403 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6489000e+00 -3.0911000e-04 -2.1515000e-04 /
CHEB / 2.2353000e+00 3.9766000e-04 2.7678000e-04 /
CHEB / 3.2345000e-01 -6.0959000e-05 -4.2426000e-05 /
CHEB / 5.0478000e-02 -3.6358000e-05 -2.5304000e-05 /
CHEB / -8.0821000e-03 5.7700000e-06 4.0120000e-06 /

tSPC(3683)+CH3(+m)=CH3+sSPC(1356)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7899000e+00 -2.2790000e-03 -1.5847000e-03 /
CHEB / 4.8064000e+00 3.0873000e-03 2.1463000e-03 /
CHEB / 2.5884000e-01 -7.3344000e-04 -5.0908000e-04 /
CHEB / 9.8791000e-03 -1.2812000e-04 -8.9566000e-05 /
CHEB / -3.3198000e-02 4.0864000e-05 2.8362000e-05 /

tSPC(3683)+CH3(+m)=acetone+nSPC(102)(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
14.177848957422192 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4627000e+00 -1.1130000e-03 -7.7839000e-04 /
CHEB / 3.3497000e+00 1.6142000e-03 1.1294000e-03 /
CHEB / -1.2890000e-01 -5.0765000e-04 -3.5597000e-04 /
CHEB / -1.0206000e-01 -5.9317000e-05 -4.0879000e-05 /
CHEB / -6.5728000e-02 7.3251000e-05 5.1159000e-05 /

C4H8O2(62)+O(+m)=tSPC(3683)+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O3JJ(334))      deltaHrxn(T=298K) = -
23.49777943257434 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0695000e+01 -1.7697000e-04 -1.2327000e-04 /
CHEB / 1.0649000e+00 2.1752000e-04 1.5152000e-04 /
CHEB / 3.7611000e-02 -1.5663000e-05 -1.0936000e-05 /
CHEB / -2.6047000e-02 -3.0877000e-05 -2.1501000e-05 /
CHEB / -3.3600000e-02 3.4585000e-06 2.4149000e-06 /
```

```
CH2+sSPC(1474)(+m)=tSPC(3683)+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
11.828688945695937 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6100000e+00 -1.0652000e-03 -7.4070000e-04 /
CHEB / 2.0940000e+00 1.4970000e-03 1.0408000e-03 /
CHEB / 6.2625000e-02 -4.2237000e-04 -2.9341000e-04 /
CHEB / 6.7869000e-03 -4.6927000e-05 -3.2780000e-05 /
CHEB / -3.9739000e-03 3.5091000e-05 2.4362000e-05 /

CH3+sSPC(1356)(+m)=CH2C[O]CH3+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) =
4.399785650573541 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4789000e+00 -3.6569000e-03 -2.5390000e-03 /
CHEB / 6.9503000e+00 4.9583000e-03 3.4412000e-03 /
CHEB / 2.8614000e-01 -1.1161000e-03 -7.7209000e-04 /
CHEB / 4.7714000e-02 -3.1541000e-04 -2.2053000e-04 /
CHEB / -2.0928000e-02 8.7414000e-05 6.0628000e-05 /

acetone+nSPC(102)(+m)=CH2C[O]CH3+CH2OOH(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H8O3JJ(334))
      deltaHrxn(T=298K) = 8.958767847808328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3650000e+00 -3.1095000e-03 -2.1580000e-03 /
CHEB / 7.1762000e+00 4.4564000e-03 3.0910000e-03 /
CHEB / -4.5215000e-02 -1.3139000e-03 -9.0838000e-04 /
CHEB / -5.4542000e-02 -2.2315000e-04 -1.5675000e-04 /
CHEB / -6.2060000e-02 1.8756000e-04 1.2981000e-04 /

C4H8O2(62)+O(+m)=CH2C[O]CH3+CH2OOH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
28.7168605421882 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0883000e+01 -1.2008000e-07 -1.5641000e-07 /
CHEB / 9.0269000e-01 -3.8374000e-06 -2.5739000e-06 /
CHEB / -2.9760000e-02 9.6076000e-06 6.6732000e-06 /
CHEB / -3.2587000e-02 -6.8526000e-06 -4.7885000e-06 /
CHEB / -3.1520000e-02 2.9950000e-07 2.1656000e-07 /

CH2+sSPC(1474)(+m)=CH2C[O]CH3+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
17.047770055309797 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0094000e+01 -6.0433000e-04 -4.2154000e-04 /
CHEB / 1.6452000e+00 8.3712000e-04 5.8405000e-04 /
CHEB / -4.1823000e-03 -2.0130000e-04 -1.4069000e-04 /
CHEB / 4.8385000e-03 -7.1579000e-05 -4.9748000e-05 /
CHEB / -8.5283000e-04 4.1539000e-05 2.8943000e-05 /
```

```
tSPC(3683)+CH3(+m)=CH2C[O]CH3+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H8O3JJ(334)) deltaHrxn(T=298K) = -
5.21908110961386 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.6751000e+00 -1.9462000e-03 -1.3523000e-03 /
CHEB / 3.5294000e+00 2.7898000e-03 1.9381000e-03 /
CHEB / -8.5316000e-02 -8.5984000e-04 -5.9644000e-04 /
CHEB / -5.3103000e-02 -5.7444000e-05 -4.0559000e-05 /
CHEB / -2.5073000e-02 6.9082000e-05 4.8000000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+CH3(+m)=CH3O+iC4H7(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1589 (C5H10O(2615))    deltaHrxn(T=298K) = -
12.038337009634063 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0999000e+01 -1.3768000e+00 -5.7603000e-02 /
CHEB / 2.1396000e+00 1.0024000e+00 -5.7194000e-02 /
CHEB / 3.4703000e-01 4.8844000e-01 3.7344000e-02 /
CHEB / -1.9272000e-01 6.5668000e-02 6.9094000e-02 /
CHEB / -1.4914000e-01 -1.0462000e-01 3.5437000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
```

```
!     sSPC(1697)  4.3   64.82 13.25 15.03 16.62 18.2  20.78 23.21 26.73
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1697)+sC3H5(+m)=CH3O+CH2C[O]CH3(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1767 (C4H8O2(2725))     deltaHrxn(T=298K) = -
64.58334076405288 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2722000e+01 -9.8933000e-06 -6.8864000e-06 /
CHEB / -6.5667000e-02 -9.9003000e-06 -6.8912000e-06 /
CHEB / -2.8564000e-02 -6.8122000e-06 -4.7417000e-06 /
CHEB / -1.3521000e-03 -6.3227000e-06 -4.4010000e-06 /
CHEB / -7.0008000e-03 -4.8785000e-06 -3.3958000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+tSPC(3683)(+m)=CO2+sSPC(1474)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H6O5(335))  deltaHrxn(T=298K)
= -103.02904509258644 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2629000e+00 -8.8198000e-02 -6.0156000e-02 /
CHEB / 3.7656000e-01 1.1191000e-01 7.5530000e-02 /
CHEB / 2.9344000e-01 -1.0774000e-02 -6.0791000e-03 /
CHEB / 1.1096000e-01 -1.6556000e-02 -1.1404000e-02 /
CHEB / 3.5217000e-02 5.5538000e-05 -5.2837000e-04 /

!PDepNetwork
```

```
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+CH2C[O]CH3(+m)=iC4H7+sSPC(1474)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #8 (C7H13O3J(436))
      deltaHrxn(T=298K) = -11.188343209493638 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7637000e+00 -1.9054000e-01 -1.1336000e-01 /
CHEB / 1.5453000e+01 1.7899000e-01 1.0045000e-01 /
CHEB / 2.6329000e-03 -3.6519000e-03 4.0785000e-03 /
CHEB / -8.7658000e-02 1.0841000e-02 6.0226000e-03 /
CHEB / -4.5658000e-02 1.3962000e-02 7.9475000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
```

```
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     sSPC(1474)  -67.94      85.82 28.37 33.77 38.22 41.77 46.97 50.61
      56.09
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+tSPC(3683)(+m)=tSPC(77)+sSPC(1474)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = -10.66908623199842 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0709000e+00 -2.0154000e-01 -1.0925000e-01 /
CHEB / 1.6615000e+01 2.5082000e-01 1.3155000e-01 /
CHEB / 2.4596000e-02 -1.9425000e-02 -3.7179000e-03 /
CHEB / -2.0800000e-01 -3.3975000e-02 -1.9207000e-02 /
CHEB / -9.6219000e-02 -4.0341000e-03 -4.3773000e-03 /

C4H8O2(62)+tSPC(3683)(+m)=C4H8O2(62)+sSPC(1356)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = -9.618866760187405 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0651000e+01 -7.6265000e-01 -2.8838000e-01 /
CHEB / 1.6980000e+01 9.6682000e-01 3.2369000e-01 /
CHEB / -2.3325000e-01 -1.0061000e-01 3.1351000e-02 /
CHEB / -3.5604000e-01 -1.2478000e-01 -6.2388000e-02 /
CHEB / -1.2729000e-01 -7.3119000e-03 -2.3458000e-02 /

C4H8O2(62)+sSPC(1356)(+m)=tSPC(77)+sSPC(1474)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = -1.050219471811019 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1640000e+01 -9.0322000e-01 -2.8529000e-01 /
CHEB / 1.8414000e+01 1.1222000e+00 2.9676000e-01 /
CHEB / -2.1978000e-01 -8.2766000e-02 6.6868000e-02 /
CHEB / -3.6449000e-01 -1.5204000e-01 -6.4970000e-02 /
CHEB / -1.3594000e-01 -2.3474000e-02 -3.4539000e-02 /

C4H8O2(62)+tSPC(3683)(+m)=tSPC(54)+sSPC(1474)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = -10.668912399179959 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7221000e+00 -7.8254000e-01 -2.9115000e-01 /
CHEB / 1.6391000e+01 9.8409000e-01 3.2328000e-01 /
CHEB / -3.0810000e-01 -8.7925000e-02 3.6985000e-02 /
```

```
CHEB / -3.6945000e-01 -1.3510000e-01 -6.2992000e-02 /
CHEB / -1.3925000e-01 -9.7888000e-03 -2.5997000e-02 /

tSPC(54)+sSPC(1474)(+m)=tSPC(77)+sSPC(1474)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = -1.7383281846150567E-4 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0813000e+01 -9.6282000e-01 -2.7880000e-01 /
CHEB / 1.7916000e+01 1.1929000e+00 2.7938000e-01 /
CHEB / -2.4677000e-01 -8.4975000e-02 8.1945000e-02 /
CHEB / -3.8762000e-01 -1.5806000e-01 -6.5619000e-02 /
CHEB / -1.3808000e-01 -2.9814000e-02 -3.8747000e-02 /

tSPC(54)+sSPC(1474)(+m)=C4H8O2(62)+sSPC(1356)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H13O5J(364))
      deltaHrxn(T=298K) = 1.0500456389925539 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0652000e+01 -7.1043000e-01 -1.7013000e-01 /
CHEB / 1.8146000e+01 8.7573000e-01 1.5456000e-01 /
CHEB / 1.1176000e-02 -5.1078000e-02 7.6583000e-02 /
CHEB / -1.6660000e-01 -1.2494000e-01 -4.4875000e-02 /
CHEB / -4.5387000e-02 -2.3396000e-02 -3.3227000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+sSPC(2810)(+m)=CH2CHO+sSPC(1474)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #29 (C5H9O4J(555))
      deltaHrxn(T=298K) = -1.8092798174012188 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -1.1242000e+01 -2.2260000e-06 -1.5494000e-06 /
CHEB / 1.8249000e+01 -1.9362000e-07 -1.3477000e-07 /
CHEB / 5.1713000e-01 2.0790000e-06 1.4472000e-06 /
CHEB / 6.0327000e-02 8.7560000e-07 6.0948000e-07 /
CHEB / -3.2392000e-02 -1.8874000e-07 -1.3137000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+sC3H5(+m)=C4H7OJ(79)+CH2C[O]CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #79 (C7H12O2(1053))
      deltaHrxn(T=298K) = -64.79335487624601 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3089000e+01 -1.8204000e-04 -1.2667000e-04 /
CHEB / -3.6837000e-01 -2.8431000e-04 -1.9781000e-04 /
CHEB / -2.8687000e-02 -2.4162000e-04 -1.6810000e-04 /
CHEB / -1.4508000e-03 -1.9610000e-04 -1.3642000e-04 /
CHEB / -7.0707000e-03 -1.4197000e-04 -9.8759000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
```

```
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+CH2C[O]CH3(+m)=iC4H7+sSPC(1590)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #126 (C7H12O2JJ(968))
      deltaHrxn(T=298K) = -11.18834333136044 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3883000e+00 -3.3149000e-04 -2.3068000e-04 /
CHEB / 1.6311000e+01 4.1626000e-04 2.8966000e-04 /
CHEB / 3.9138000e-01 -5.9859000e-05 -4.1629000e-05 /
CHEB / 1.0841000e-01 -1.9360000e-05 -1.3485000e-05 /
CHEB / -3.2156000e-02 -1.5164000e-05 -1.0551000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(1356)  -32.36      90.0  21.79 28.09 32.24 35.76 41.27 45.47
      50.74 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(1356)+sC3H5(+m)=sSPC(1590)+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #160 (C6H10O3(953))
      deltaHrxn(T=298K) = -64.79335493959184 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3243000e+01 4.3013000e-10 2.9940000e-10 /
CHEB / -4.9544000e-01 8.4102000e-10 5.8542000e-10 /
CHEB / -2.8749000e-02 7.8499000e-10 5.4641000e-10 /
CHEB / -1.5205000e-03 6.9678000e-10 4.8501000e-10 /
CHEB / -7.1462000e-03 5.8291000e-10 4.0575000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     sSPC(1590)  -30.7 78.33 21.08 25.77 29.92 33.34 38.35 41.79 46.82
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     sSPC(1356)  -30.79      86.93 25.24 29.96 34.0  37.3  42.29 45.86
      51.26
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+tSPC(3683)(+m)=sSPC(1590)+tSPC(77)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = -9.18901159167931 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0585000e+01 -3.8337000e-04 -2.6677000e-04 /
CHEB / 1.7210000e+01 4.7473000e-04 3.3033000e-04 /
CHEB / 5.3291000e-01 -5.1234000e-05 -3.5623000e-05 /
CHEB / 1.0876000e-01 -4.3982000e-05 -3.0612000e-05 /
CHEB / -6.8121000e-02 -4.7147000e-06 -3.2851000e-06 /

C4H7OJ(79)+tSPC(3683)(+m)=tSPC(54)+sSPC(1590)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = -9.188837758860853 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8517000e+01 -1.2965000e-03 -9.0193000e-04 /
CHEB / 2.1211000e+01 1.6190000e-03 1.1261000e-03 /
CHEB / 1.3591000e+00 -1.6514000e-04 -1.1472000e-04 /
CHEB / 2.3651000e-01 -2.1419000e-04 -1.4900000e-04 /
CHEB / -6.2696000e-02 4.5514000e-05 3.1612000e-05 /
```

```
tSPC(54)+sSPC(1590)(+m)=sSPC(1590)+tSPC(77)(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = -1.7383281845795295E-4 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9414000e+01 -2.4196000e-03 -1.6803000e-03 /
CHEB / 2.2522000e+01 3.2817000e-03 2.2780000e-03 /
CHEB / 1.3956000e+00 -7.9841000e-04 -5.5274000e-04 /
CHEB / 2.3419000e-01 -1.0248000e-04 -7.1918000e-05 /
CHEB / -3.1026000e-02 7.5782000e-06 5.0547000e-06 /

C4H7OJ(79)+tSPC(3683)(+m)=sSPC(1356)+C4H7OJ(79)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = -9.618866760187402 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7534000e+01 -1.3011000e-03 -9.0521000e-04 /
CHEB / 2.0538000e+01 1.6215000e-03 1.1280000e-03 /
CHEB / 1.2647000e+00 -1.5989000e-04 -1.1106000e-04 /
CHEB / 2.2742000e-01 -2.1036000e-04 -1.4642000e-04 /
CHEB / -6.9965000e-02 2.7386000e-05 1.9047000e-05 /

sSPC(1356)+C4H7OJ(79)(+m)=sSPC(1590)+tSPC(77)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = 0.4298551685080909 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8358000e+01 -2.8753000e-03 -1.9958000e-03 /
CHEB / 2.1815000e+01 3.9664000e-03 2.7519000e-03 /
CHEB / 1.3747000e+00 -1.0446000e-03 -7.2280000e-04 /
CHEB / 2.2874000e-01 -1.3101000e-04 -9.1959000e-05 /
CHEB / -2.6973000e-02 8.1431000e-05 5.6206000e-05 /

sSPC(1356)+C4H7OJ(79)(+m)=tSPC(54)+sSPC(1590)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C7H12O4JJ(378))
      deltaHrxn(T=298K) = 0.43002900132654887 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2149000e+01 -3.5593000e-03 -2.4664000e-03 /
CHEB / 1.8758000e+01 4.7586000e-03 3.2953000e-03 /
CHEB / 6.1952000e-01 -9.4663000e-04 -6.5211000e-04 /
CHEB / 1.0366000e-01 -3.9667000e-04 -2.7632000e-04 /
CHEB / -1.4088000e-02 8.7450000e-05 5.9926000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
```

```
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5            61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3071)+iC4H7(+m)=C4H7OJ(79)+sSPC(2810)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #627 (C5H8O3(1049))
      deltaHrxn(T=298K) = -31.506743221791535 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3252000e+01 -1.0195000e-01 -6.5302000e-02 /
CHEB / -5.1371000e-01 6.5355000e-02 4.1197000e-02 /
CHEB / -1.6345000e-02 2.2073000e-02 1.3221000e-02 /
CHEB / -1.0744000e-02 -1.6920000e-02 -1.0232000e-02 /
CHEB / -1.0507000e-02 -8.7261000e-03 -5.3948000e-03 /

tSPC(54)+HCO(+m)=sSPC(3071)+iC4H7(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #627 (C5H8O3(1049))      deltaHrxn(T=298K) = -
17.52793665811422 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9978000e+00 -1.4472000e-02 -9.9758000e-03 /
CHEB / 1.8262000e+00 3.1203000e-03 2.1659000e-03 /
CHEB / 7.9594000e-01 2.7348000e-04 1.8928000e-04 /
CHEB / 2.3686000e-01 -4.2431000e-03 -2.9032000e-03 /
CHEB / 4.4195000e-02 -2.1993000e-03 -1.5027000e-03 /

tSPC(54)+HCO(+m)=C4H7OJ(79)+sSPC(2810)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #627 (C5H8O3(1049))
      deltaHrxn(T=298K) = -49.03467987990575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3283000e+01 -1.9619000e-02 -1.3469000e-02 /
CHEB / -5.2051000e-01 4.8926000e-05 1.0955000e-04 /
CHEB / -2.4648000e-02 1.0248000e-03 7.2783000e-04 /
CHEB / 1.2412000e-02 -4.4086000e-03 -2.9924000e-03 /
CHEB / 6.3487000e-04 -2.8171000e-03 -1.9096000e-03 /

sSPC(3071)+iC4H7(+m)=C4H8O2(62)+CO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #627 (C5H8O3(1049))      deltaHrxn(T=298K) = -
55.384822817371415 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8899000e+00 -5.9533000e-02 -3.9312000e-02 /
```

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CHEB / 4.6088000e+00 4.7472000e-02 3.0831000e-02 /
CHEB / 1.2840000e+00 2.6641000e-03 1.6938000e-03 /
CHEB / 3.2918000e-01 -1.3067000e-02 -8.3968000e-03 /
CHEB / 8.3055000e-02 -3.4317000e-03 -2.3487000e-03 /

C4H7OJ(79)+sSPC(2810)(+m)=C4H8O2(62)+CO(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #627 (C5H8O3(1049))
      deltaHrxn(T=298K) = -23.878079595579877 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5336000e+00 -1.3231000e-01 -8.2238000e-02 /
CHEB / 1.1349000e+01 9.3499000e-02 5.6746000e-02 /
CHEB / 5.6773000e-01 2.7527000e-02 1.5871000e-02 /
CHEB / 1.9491000e-01 -2.1367000e-02 -1.2230000e-02 /
CHEB / 7.6183000e-02 -1.0495000e-02 -6.2990000e-03 /

tSPC(54)+HCO(+m)=C4H8O2(62)+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #627 (C5H8O3(1049))     deltaHrxn(T=298K) = -
72.91275947548563 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3055000e+00 -1.4985000e-02 -1.0325000e-02 /
CHEB / 3.3583000e+00 3.0100000e-03 2.0920000e-03 /
CHEB / 1.1930000e+00 4.4789000e-04 3.0931000e-04 /
CHEB / 3.8816000e-01 -4.2974000e-03 -2.9386000e-03 /
CHEB / 1.0796000e-01 -2.2970000e-03 -1.5683000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!Here are the path reactions and their high-P limit kinetics:

HCO+tSPC(77)(+m)=CO+C4H8O2(62)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #736 (C5H8O3(1227))     deltaHrxn(T=298K) = -
72.91258564266718 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 2.4734000e+00 -7.0664000e-02 -4.5334000e-02 /
CHEB / 6.7902000e+00 8.8945000e-02 5.6478000e-02 /
CHEB / 8.1938000e-01 -9.1437000e-03 -5.0256000e-03 /
CHEB / 2.2878000e-01 -1.2423000e-02 -8.0354000e-03 /
CHEB / 6.1822000e-02 2.4747000e-04 -1.6115000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tBuOH       -75.1 78.01 27.2  34.21 40.27 45.3  53.28 59.16 68.42
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

HCO+HOC[CH2][CH3]2(+m)=CH2CHO+CH3C[OH]CH3(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1744 (C5H10O2(1257))
      deltaHrxn(T=298K) = -1.1097755337137833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4307000e+00 -1.3649000e+00 -4.6456000e-02 /
CHEB / 3.4823000e+00 1.0366000e+00 -4.4733000e-02 /
CHEB / 2.8017000e-01 5.1886000e-01 4.1011000e-02 /
CHEB / -3.5109000e-01 6.3744000e-02 7.2663000e-02 /
CHEB / -2.2519000e-01 -1.3550000e-01 3.4754000e-02 /

HCO+HOC[CH2][CH3]2(+m)=CO+tBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1744 (C5H10O2(1257))   deltaHrxn(T=298K) = -
85.81127316744455 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5285000e+00 -1.3649000e+00 -4.6456000e-02 /
CHEB / 4.9223000e+00 1.0366000e+00 -4.4733000e-02 /
CHEB / 6.5862000e-01 5.1886000e-01 4.1011000e-02 /
CHEB / -2.1851000e-01 6.3744000e-02 7.2663000e-02 /
CHEB / -1.7301000e-01 -1.3550000e-01 3.4754000e-02 /
```

```
CH2CHO+CH3C[OH]CH3(+m)=CO+tBuOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1744 (C5H10O2(1257))   deltaHrxn(T=298K) = -
84.70149763373077 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.1650000e+00 -1.3649000e+00 -4.6456000e-02 /
CHEB / 4.9719000e+00 1.0366000e+00 -4.4733000e-02 /
CHEB / 5.3840000e-01 5.1886000e-01 4.1011000e-02 /
CHEB / -2.8462000e-01 6.3744000e-02 7.2663000e-02 /
CHEB / -2.1445000e-01 -1.3550000e-01 3.4754000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sC3H5+CH2CHO(+m)=iC4H7+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1908 (C5H8O(1132))     deltaHrxn(T=298K) = -
25.13773838843268 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2603000e+01 -6.3171000e-01 -2.1309000e-01 /
CHEB / 7.0000000e-02 6.2846000e-01 1.8069000e-01 /
CHEB / 7.4993000e-03 1.1613000e-01 6.6582000e-02 /
CHEB / -8.7416000e-02 -6.6953000e-02 -5.1002000e-03 /
CHEB / -6.4842000e-02 -4.9389000e-02 -2.3222000e-02 /

sC3H5+CH2CHO(+m)=iC4H8+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1908 (C5H8O(1132))     deltaHrxn(T=298K) = -
98.05032399118458 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2048000e+00 -5.6958000e-01 -2.0202000e-01 /
CHEB / 2.1528000e+00 6.0739000e-01 1.8592000e-01 /
CHEB / 5.8685000e-01 6.2135000e-02 5.4529000e-02 /
CHEB / 8.5959000e-02 -7.1159000e-02 -1.5572000e-02 /
CHEB / 1.8131000e-03 -3.9349000e-02 -2.3211000e-02 /
```

```
iC4H7+HCO(+m)=iC4H8+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1908 (C5H8O(1132))     deltaHrxn(T=298K) = -
72.9125856027519 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6985000e+00 -1.0550000e+00 -1.3571000e-01 /
CHEB / 6.1691000e+00 9.9416000e-01 4.2507000e-02 /
CHEB / 3.4107000e-01 2.3059000e-01 1.0143000e-01 /
CHEB / -1.6081000e-02 -7.0332000e-02 3.3341000e-02 /
CHEB / -2.5343000e-02 -8.7040000e-02 -1.9311000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+sC3H5(+m)=CH3+iC4H5OJ(14)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C5H8O(1180))     deltaHrxn(T=298K) = -
20.898512973282678 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1605000e+01 -1.1970000e+00 -1.1829000e-01 /
CHEB / 9.2566000e-01 9.9969000e-01 -6.3894000e-03 /
CHEB / 1.3779000e-01 3.3817000e-01 9.1075000e-02 /
CHEB / -1.1769000e-01 -1.6221000e-02 5.9533000e-02 /
CHEB / -9.0970000e-02 -9.2068000e-02 1.7790000e-03 /

CH3+iC4H5OJ(14)(+m)=iC4H8+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C5H8O(1180))     deltaHrxn(T=298K) = -
68.58264086496307 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8738000e+00 -8.0701000e-01 -2.1780000e-01 /
CHEB / 1.3646000e+01 7.4097000e-01 1.4633000e-01 /
CHEB / 3.5843000e-01 1.8781000e-01 8.9627000e-02 /
CHEB / 8.2302000e-02 -5.0812000e-02 1.6073000e-02 /
CHEB / 2.1140000e-02 -6.5354000e-02 -2.0709000e-02 /
```

```
CH3CO+sC3H5(+m)=iC4H8+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2307 (C5H8O(1180))     deltaHrxn(T=298K) = -
89.48115383824575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.6441000e+00 -7.3760000e-01 -2.1070000e-01 /
CHEB / 7.6423000e+00 7.3716000e-01 1.6140000e-01 /
CHEB / 7.6154000e-01 1.2578000e-01 8.3013000e-02 /
CHEB / 1.5156000e-01 -7.2624000e-02 -7.0376000e-04 /
CHEB / 3.3738000e-02 -6.0271000e-02 -2.6769000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

HCO+H2CCCO(+m)=CO+tSPC(346)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2684 (C4H3O2J(1631))   deltaHrxn(T=298K) = -
49.89601858897245 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8191000e+00 -5.8474000e-01 -2.0638000e-01 /
CHEB / 7.9292000e+00 6.3011000e-01 1.8323000e-01 /
CHEB / 1.9250000e-01 3.2448000e-02 5.3244000e-02 /
CHEB / 5.4674000e-02 -7.0484000e-02 -1.7766000e-02 /
CHEB / 4.3255000e-02 -2.3536000e-02 -1.7810000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!Here are the path reactions and their high-P limit kinetics:

H2CCCO+HCO(+m)=C3H3O-enone+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3095 (C4H3O2J(1671))   deltaHrxn(T=298K) = -
66.69425718312525 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7486000e+00 -4.4932000e-04 -3.1266000e-04 /
CHEB / 5.6502000e+00 4.0390000e-04 2.8103000e-04 /
CHEB / 9.5465000e-01 7.4026000e-05 5.1529000e-05 /
CHEB / 2.9686000e-01 -1.9420000e-05 -1.3501000e-05 /
CHEB / 9.2322000e-02 -1.4785000e-05 -1.0290000e-05 /

CO+tSPC(346)(+m)=C3H3O-enone+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3095 (C4H3O2J(1671))   deltaHrxn(T=298K) = -
16.798238594152792 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1762000e+01 4.6670000e-07 3.2485000e-07 /
CHEB / 1.9752000e+01 8.1085000e-07 5.6440000e-07 /
CHEB / 2.3648000e-01 5.9332000e-07 4.1299000e-07 /
CHEB / 8.2149000e-02 3.8986000e-07 2.7137000e-07 /
CHEB / 2.6445000e-02 2.3703000e-07 1.6499000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!Here are the path reactions and their high-P limit kinetics:

HCO+tSPC(3683)(+m)=CO+sSPC(1474)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3676 (C4H6O4(1214))     deltaHrxn(T=298K) = -
84.10092885383533 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2414000e+00 -1.8439000e-02 -1.2558000e-02 /
CHEB / 4.6385000e+00 2.4761000e-02 1.6815000e-02 /
CHEB / 1.0925000e+00 -5.0077000e-03 -3.3238000e-03 /
CHEB / 2.8257000e-01 -2.1424000e-03 -1.4918000e-03 /
CHEB / 5.5611000e-02 5.1381000e-04 3.3609000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!Here are the path reactions and their high-P limit kinetics:

CH2CO+sC3H5(+m)=CO+iC4H7(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3970 (C5H7OJ(1250))    deltaHrxn(T=298K) = -
44.32570741874123 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0592000e+00 7.1851000e-08 5.0013000e-08 /
CHEB / 2.8586000e+00 1.3854000e-07 9.6433000e-08 /
CHEB / 1.2988000e-01 1.2414000e-07 8.6413000e-08 /
CHEB / 3.1691000e-02 1.0336000e-07 7.1948000e-08 /
CHEB / -1.2526000e-02 7.9758000e-08 5.5517000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!Here are the path reactions and their high-P limit kinetics:

CO+tSPC(54)(+m)=CO2+C4H7OJ(79)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4197 (C5H7O3J(997))    deltaHrxn(T=298K) = -
67.96279611865688 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0852000e+00 5.8852000e-16 -6.5251000e-16 /
CHEB / 2.0705000e+00 -1.5382000e-15 1.0551000e-15 /
CHEB / -6.9823000e-01 1.1354000e-15 -1.0817000e-15 /
CHEB / -8.8164000e-03 -9.6197000e-16 8.7663000e-16 /
CHEB / 4.9233000e-02 8.9017000e-16 -5.4248000e-16 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+tSPC(110)(+m)=sSPC(2810)+C4H6Oi-13(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4485 (C5H7O3J(1061))
      deltaHrxn(T=298K) = -53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3487000e+01 -1.4246000e-03 -9.9049000e-04 /
CHEB / -9.7666000e-01 -7.8583000e-04 -5.4552000e-04 /
CHEB / -1.7875000e-01 -4.4477000e-04 -3.0853000e-04 /
CHEB / -1.1693000e-01 -3.9205000e-04 -2.7210000e-04 /
CHEB / -7.6392000e-02 -1.3645000e-04 -9.4575000e-05 /
```

```
sSPC(2810)+C4H6Oi-13(+m)=CO2+C4H7OJ(79)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4485 (C5H7O3J(1061))
      deltaHrxn(T=298K) = -14.70845361967067 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3299000e+01 -1.1294000e-03 -7.8544000e-04 /
CHEB / 2.0761000e+01 -7.2617000e-04 -5.0443000e-04 /
CHEB / 6.1434000e-02 -4.0592000e-04 -2.8179000e-04 /
CHEB / -1.9604000e-02 -3.2843000e-04 -2.2807000e-04 /
CHEB / -2.8034000e-02 -1.1769000e-04 -8.1641000e-05 /

sSPC(2810)+tSPC(110)(+m)=CO2+C4H7OJ(79)(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #4485 (C5H7O3J(1061))
      deltaHrxn(T=298K) = -68.11305289765136 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0226000e+00 -8.1212000e-04 -5.6499000e-04 /
CHEB / 5.8039000e+00 -3.4719000e-04 -2.4134000e-04 /
CHEB / 9.2878000e-01 -2.0539000e-04 -1.4274000e-04 /
CHEB / 1.8849000e-01 -2.1046000e-04 -1.4631000e-04 /
CHEB / 8.0678000e-03 -8.0687000e-05 -5.6076000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!Here are the path reactions and their high-P limit kinetics:

CO+CH2C[O]CH3(+m)=CO2+sC3H5(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4815 (C4H5O2J(1097))   deltaHrxn(T=298K) = -
3.169441242410855 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2932000e+00 -7.4235000e-06 -5.1672000e-06 /
CHEB / 1.0185000e+00 -1.4432000e-05 -1.0046000e-05 /
CHEB / 5.2049000e-04 -1.3249000e-05 -9.2219000e-06 /
CHEB / -3.1499000e-03 -1.1461000e-05 -7.9775000e-06 /
CHEB / -1.7167000e-03 -9.2871000e-06 -6.4643000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H5OJ(8)         -7.6  73.85 18.59 21.98 24.96 27.55 32.16 35.44
      39.21 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+CH2CO(+m)=CH2CO+CH3CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5243 (C4H5O2J(1223))   deltaHrxn(T=298K) = -
8.569170152938833 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6330000e+00 -8.5719000e-01 -1.4921000e-01 /
CHEB / 6.0491000e+00 9.4792000e-01 9.2695000e-02 /
CHEB / 3.0149000e-01 5.4574000e-02 9.8930000e-02 /
CHEB / -8.6477000e-02 -1.0753000e-01 -5.3801000e-03 /
CHEB / -7.9758000e-02 -5.2310000e-02 -3.1094000e-02 /

CH2CHO+CH2CO(+m)=C3H5OJ(8)+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5243 (C4H5O2J(1223))   deltaHrxn(T=298K) = -
28.967383322476344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3480000e+01 1.6772000e-04 1.1607000e-04 /
CHEB / 2.8622000e+01 -3.9782000e-05 -2.7011000e-05 /
CHEB / 4.0831000e-01 -8.5076000e-05 -5.9061000e-05 /
CHEB / 6.2952000e-02 -5.4489000e-05 -3.8053000e-05 /
CHEB / -3.2653000e-02 -7.8995000e-06 -5.5771000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
```

```
!     iC4H8       -3.8  69.99 21.58 26.65 31.3  35.34 41.91 46.89 54.71
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H9       16.5  76.33 22.57 28.26 33.45 37.96 45.1  50.52 60.07
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+CH3(+m)=iC4H8+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
0.8696209845508704 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3384000e+00 -2.5594000e-01 -1.2299000e-01 /
CHEB / 3.6798000e+00 3.0942000e-01 1.4275000e-01 /
CHEB / -4.5175000e-02 -1.7130000e-02 -1.7413000e-03 /
CHEB / -1.0802000e-02 -4.2604000e-02 -1.8256000e-02 /
CHEB / 5.5872000e-03 -3.8885000e-03 -5.1331000e-03 /

tSPC(110)+CH3(+m)=C4H6Oi-13+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1553000e+01 -1.2811000e-03 -8.9105000e-04 /
CHEB / 4.9208000e-01 5.8462000e-04 4.0656000e-04 /
CHEB / 1.2857000e-01 3.6145000e-04 2.5125000e-04 /
CHEB / 6.0154000e-02 -2.0661000e-04 -1.4363000e-04 /
CHEB / 1.1443000e-02 -2.1715000e-04 -1.5096000e-04 /

tSPC(110)+CH3(+m)=iC4H8+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
54.27422026253156 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2676000e+01 -1.3068000e-03 -9.0892000e-04 /
CHEB / -1.2762000e-01 5.6911000e-04 3.9577000e-04 /
CHEB / -7.1845000e-02 3.7063000e-04 2.5763000e-04 /
CHEB / -1.0405000e-02 -2.0517000e-04 -1.4263000e-04 /
CHEB / -1.3685000e-02 -2.2283000e-04 -1.5491000e-04 /

C4H6Oi-13+CH3(+m)=iC4H9+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
17.387857043963127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2249000e+01 -1.1032000e-03 -7.6743000e-04 /
CHEB / 2.0254000e+01 4.5459000e-04 3.1618000e-04 /
CHEB / 3.4587000e-01 2.9770000e-04 2.0698000e-04 /
CHEB / 1.4950000e-01 -1.7889000e-04 -1.2439000e-04 /
CHEB / 5.5077000e-02 -1.9288000e-04 -1.3412000e-04 /
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iC4H8+HCO(+m)=iC4H9+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
16.518236059412256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1898000e+01 -1.1241000e-03 -7.8192000e-04 /
CHEB / 2.0207000e+01 4.4033000e-04 3.0626000e-04 /
CHEB / 2.4609000e-01 3.0327000e-04 2.1085000e-04 /
CHEB / 9.1410000e-02 -1.7830000e-04 -1.2397000e-04 /
CHEB / 2.8074000e-02 -1.9749000e-04 -1.3732000e-04 /

tSPC(110)+CH3(+m)=iC4H9+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6734 (C5H9OJ(1407))    deltaHrxn(T=298K) = -
70.7924563219438 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3432000e+00 -7.5855000e-04 -5.2777000e-04 /
CHEB / 5.5908000e+00 4.1954000e-04 2.9185000e-04 /
CHEB / 1.2234000e+00 1.2616000e-04 8.7750000e-05 /
CHEB / 3.2934000e-01 -1.4543000e-04 -1.0115000e-04 /
CHEB / 8.1063000e-02 -1.1679000e-04 -8.1247000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     C4H6O(105)  -2.12 71.03 19.46 26.19 31.81 36.09 42.58 47.31 53.93
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:

C4H6O(105)+OH(+m)=C4H6Oi-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) = -
25.218118470884093 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9160000e+00 1.2322000e-12 8.5676000e-13 /
CHEB / 1.5495000e+01 2.4142000e-12 1.6822000e-12 /
CHEB / 1.8398000e-01 2.2737000e-12 1.5826000e-12 /
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CHEB / 4.3225000e-02 2.0452000e-12 1.4220000e-12 /
CHEB / 1.0932000e-02 1.7344000e-12 1.2103000e-12 /

tSPC(110)+OH(+m)=C4H6O(105)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) = -
28.186480807096594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0118000e+01 -1.8284000e-10 -1.2727000e-10 /
CHEB / 1.5935000e+01 -3.5172000e-10 -2.4482000e-10 /
CHEB / 6.8528000e-01 -3.1282000e-10 -2.1774000e-10 /
CHEB / 2.0243000e-01 -2.5687000e-10 -1.7880000e-10 /
CHEB / 6.9809000e-02 -1.9404000e-10 -1.3506000e-10 /

C4H6Oi-13+OH(+m)=tSPC(77)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) = 32.0570081526085
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5852000e+01 1.0145000e-12 7.0538000e-13 /
CHEB / 2.2323000e+01 1.9875000e-12 1.3851000e-12 /
CHEB / 3.5257000e-01 1.8716000e-12 1.3034000e-12 /
CHEB / 1.5075000e-01 1.6845000e-12 1.1704000e-12 /
CHEB / 6.5819000e-02 1.4269000e-12 9.9754000e-13 /

C4H6Oi-13+OH(+m)=tSPC(54)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) =
32.057181985426965 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6892000e+01 1.2316000e-12 8.5718000e-13 /
CHEB / 2.3974000e+01 2.4157000e-12 1.6808000e-12 /
CHEB / 2.2904000e-01 2.2723000e-12 1.5838000e-12 /
CHEB / 1.0743000e-01 2.0470000e-12 1.4206000e-12 /
CHEB / 4.8739000e-02 1.7327000e-12 1.2118000e-12 /

C4H6O(105)+OH(+m)=tSPC(77)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) =
6.838889681724412 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6438000e+01 -2.3372000e-10 -1.6268000e-10 /
CHEB / 2.7907000e+01 -4.4981000e-10 -3.1310000e-10 /
CHEB / 1.1693000e+00 -4.0067000e-10 -2.7889000e-10 /
CHEB / 2.9999000e-01 -3.2984000e-10 -2.2960000e-10 /
CHEB / 1.0440000e-01 -2.5008000e-10 -1.7406000e-10 /

C4H6O(105)+OH(+m)=tSPC(54)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #6875 (C4H7O2J(543))    deltaHrxn(T=298K) = 6.83906351454287
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6458000e+01 -2.6004000e-10 -1.8101000e-10 /
CHEB / 2.8510000e+01 -5.0066000e-10 -3.4850000e-10 /
CHEB / 1.1112000e+00 -4.4648000e-10 -3.1078000e-10 /
CHEB / 2.7897000e-01 -3.6828000e-10 -2.5636000e-10 /
CHEB / 9.2255000e-02 -2.8000000e-10 -1.9489000e-10 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CH[OH]CH2      -16.5 77.94 20.71 25.46 29.81 33.14 38.71 42.81
      49.45 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+OH(+m)=H2CCCH3[OH]+HCO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
10.388626743329837 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2950000e+01 -1.7380000e-01 -8.2429000e-02 /
CHEB / -4.5469000e-01 2.3415000e-01 1.0676000e-01 /
CHEB / -9.2215000e-02 -4.8495000e-02 -1.6052000e-02 /
CHEB / -2.9854000e-02 -2.0184000e-02 -1.1375000e-02 /
CHEB / -1.4778000e-02 3.9707000e-03 1.4616000e-04 /

tSPC(110)+OH(+m)=C4H6Oi-13+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7652 (C4H7O2J(2678))   deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2168000e+01 -1.4701000e-04 -1.0232000e-04 /
CHEB / -6.6720000e-02 1.9264000e-05 1.3409000e-05 /
CHEB / 1.3152000e-01 1.6349000e-05 1.1379000e-05 /
CHEB / 3.1958000e-02 -2.9883000e-05 -2.0798000e-05 /
CHEB / -1.1409000e-02 -2.6843000e-05 -1.8682000e-05 /

tSPC(110)+OH(+m)=H2CCCH3[OH]+HCO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
63.79322602131053 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.3566000e+01 -1.4847000e-04 -1.0334000e-04 /
CHEB / -9.1817000e-01 1.7945000e-05 1.2491000e-05 /
CHEB / -1.0777000e-01 1.6129000e-05 1.1226000e-05 /
CHEB / -5.2226000e-02 -3.0115000e-05 -2.0959000e-05 /
CHEB / -4.3203000e-02 -2.7150000e-05 -1.8896000e-05 /

C4H6Oi-13+OH(+m)=CH3CH[OH]CH2+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
24.897143618739996 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.5166000e+00 -1.6584000e-04 -1.1543000e-04 /
CHEB / 1.7772000e+01 3.0231000e-05 2.1041000e-05 /
CHEB / 2.9549000e-01 2.2037000e-05 1.5337000e-05 /
CHEB / 1.0246000e-01 -3.2683000e-05 -2.2746000e-05 /
CHEB / 2.4856000e-02 -2.9322000e-05 -2.0407000e-05 /

H2CCCH3[OH]+HCO(+m)=CH3CH[OH]CH2+CO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
14.508516875410159 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2818000e+01 -1.6756000e-04 -1.1663000e-04 /
CHEB / 2.0882000e+01 2.8800000e-05 2.0046000e-05 /
CHEB / 2.5896000e-01 2.1923000e-05 1.5257000e-05 /
CHEB / 8.9765000e-02 -3.2893000e-05 -2.2892000e-05 /
CHEB / 2.2835000e-02 -2.9667000e-05 -2.0647000e-05 /

tSPC(110)+OH(+m)=CH3CH[OH]CH2+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
78.30174289672068 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4537000e+00 -9.8505000e-05 -6.8563000e-05 /
CHEB / 4.4412000e+00 2.6561000e-05 1.8487000e-05 /
CHEB / 1.2496000e+00 5.3911000e-06 3.7523000e-06 /
CHEB / 2.9711000e-01 -2.2773000e-05 -1.5850000e-05 /
CHEB / 4.4575000e-02 -1.6504000e-05 -1.1487000e-05 /

C4H6Oi-13+OH(+m)=iC4H5OJ(14)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
36.21645028550476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3801000e+00 -1.2525000e-02 -8.5747000e-03 /
CHEB / 5.0246000e+00 1.4786000e-02 1.0107000e-02 /
CHEB / 5.1750000e-01 -5.0553000e-04 -3.3719000e-04 /
CHEB / 1.6880000e-01 -2.5096000e-03 -1.7046000e-03 /
CHEB / 5.1363000e-02 -1.2477000e-04 -9.6063000e-05 /

H2CCCH3[OH]+HCO(+m)=iC4H5OJ(14)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
25.827823542174926 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3499000e+00 -1.3683000e-02 -9.3585000e-03 /
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CHEB / 7.9226000e+00 1.5876000e-02 1.0844000e-02 /
CHEB / 4.4461000e-01 -7.9905000e-05 -5.0168000e-05 /
CHEB / 1.5698000e-01 -2.8635000e-03 -1.9399000e-03 /
CHEB / 5.2426000e-02 -2.4443000e-04 -1.7788000e-04 /

tSPC(110)+OH(+m)=iC4H5OJ(14)+H2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
89.62104956348546 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0661000e+00 -1.4081000e-04 -9.8007000e-05 /
CHEB / 1.5033000e+00 2.4282000e-05 1.6901000e-05 /
CHEB / 6.0667000e-01 1.6673000e-05 1.1604000e-05 /
CHEB / 1.9576000e-01 -2.9082000e-05 -2.0241000e-05 /
CHEB / 4.5822000e-02 -2.5512000e-05 -1.7756000e-05 /

CH3CH[OH]CH2+CO(+m)=iC4H5OJ(14)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #7652 (C4H7O2J(2678))    deltaHrxn(T=298K) = -
11.319306666764767 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3160000e+01 -1.5844000e-04 -1.1028000e-04 /
CHEB / 2.8184000e+01 3.5580000e-05 2.4764000e-05 /
CHEB / 9.3594000e-01 2.1781000e-05 1.5159000e-05 /
CHEB / 3.2065000e-01 -3.1973000e-05 -2.2252000e-05 /
CHEB / 1.0367000e-01 -2.7795000e-05 -1.9344000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!     sSPC(2810)  -29.51      59.94 9.81  11.32 12.68 13.78 15.39 16.47
      17.98
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(1553)  -19.27      73.08 18.28 22.22 25.51 28.12 31.86 34.37
      37.97  !MRH CBS-QB3 w/1DHR corrections
!     HCO              10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CO               -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     CO2              -94.36      50.99 8.87  9.84  10.63 11.26 12.23
      12.9  13.82
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+sSPC(2810)(+m)=tSPC(1553)+HCO(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #25 (C4H4O3JJ(358))
      deltaHrxn(T=298K) = -4.199748511132585 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6170000e+00 -3.1994000e-03 -2.2213000e-03 /
CHEB / 2.9628000e+00 3.9292000e-03 2.7267000e-03 /
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CHEB / 2.6042000e-01 -4.3771000e-04 -3.0177000e-04 /
CHEB / -4.8873000e-02 -2.8537000e-04 -1.9865000e-04 /
CHEB / -5.4366000e-02 -4.1462000e-05 -2.9073000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(122)+HCO(+m)=sSPC(3071)+tSPC(77)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #116 (C5H8O5(3240))      deltaHrxn(T=298K) = -
17.52793661924968 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3550000e+00 -6.5576000e-03 -4.5565000e-03 /
CHEB / 1.5078000e+00 6.5252000e-03 4.5336000e-03 /
CHEB / 5.0574000e-01 1.7964000e-03 1.2479000e-03 /
CHEB / 1.2968000e-01 -1.4346000e-03 -9.9564000e-04 /
CHEB / 1.2519000e-02 -7.0488000e-04 -4.8965000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
```

```
!     HOC[CH2][CH3]2    -26.1 83.61 26.43 32.85 38.36 42.9  50.12 55.42
      63.76 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(97)+HCO(+m)=sSPC(3071)+HOC[CH2][CH3]2(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #157 (C5H10O4(3243))
      deltaHrxn(T=298K) = -3.2893461656579106 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8250000e+00 -2.9845000e-02 -2.0309000e-02 /
CHEB / 4.2176000e+00 1.3788000e-02 9.3869000e-03 /
CHEB / 1.0268000e+00 -2.4841000e-03 -1.6266000e-03 /
CHEB / 1.6016000e-01 -7.5720000e-03 -5.0462000e-03 /
CHEB / -4.6491000e-02 -1.4629000e-03 -9.5781000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
!Here are the path reactions and their high-P limit kinetics:
```

```
C3H3O-enone+sSPC(3071)(+m)=tSPC(1553)+sSPC(2810)(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #304 (C4H4O4JJ(2850))
      deltaHrxn(T=298K) = -51.204475947561946 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3606000e+01 1.5153000e-06 1.0421000e-06 /
CHEB / -7.0599000e-01 3.2081000e-06 2.2201000e-06 /
CHEB / 3.2138000e-03 3.1451000e-06 2.1999000e-06 /
CHEB / 2.6121000e-02 2.7395000e-06 1.9286000e-06 /
CHEB / 5.9950000e-03 2.1369000e-06 1.4996000e-06 /

tSPC(1286)+HCO(+m)=C3H3O-enone+sSPC(3071)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #304 (C4H4O4JJ(2850))
      deltaHrxn(T=298K) = -10.398935634487152 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2482000e+00 -6.3650000e-04 -4.4289000e-04 /
CHEB / 2.2102000e+00 9.3358000e-05 6.4989000e-05 /
CHEB / 9.3020000e-01 3.6436000e-04 2.5347000e-04 /
CHEB / 2.6136000e-01 1.2575000e-04 8.7470000e-05 /
CHEB / 4.6813000e-02 -1.3047000e-05 -9.0574000e-06 /

tSPC(1286)+HCO(+m)=tSPC(1553)+sSPC(2810)(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #304 (C4H4O4JJ(2850))
      deltaHrxn(T=298K) = -61.6034115820491 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3742000e+01 3.0862000e-06 2.1478000e-06 /
CHEB / -8.9927000e-01 6.0815000e-06 4.2324000e-06 /
CHEB / -3.1845000e-02 5.5979000e-06 3.8959000e-06 /
CHEB / 8.7140000e-03 4.7955000e-06 3.3376000e-06 /
CHEB / -3.2782000e-03 3.8461000e-06 2.6768000e-06 /

C3H3O-enone+sSPC(3071)(+m)=tSPC(1416)+CO(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #304 (C4H4O4JJ(2850))
      deltaHrxn(T=298K) = -72.64280421946111 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5698000e+00 -1.0874000e-03 -7.5674000e-04 /
CHEB / 3.0504000e+00 2.1543000e-04 1.4998000e-04 /
CHEB / 1.1201000e+00 6.9268000e-04 4.8200000e-04 /
CHEB / 3.7901000e-01 2.2048000e-04 1.5339000e-04 /
CHEB / 1.1416000e-01 -6.0178000e-05 -4.1867000e-05 /

tSPC(1553)+sSPC(2810)(+m)=tSPC(1416)+CO(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #304 (C4H4O4JJ(2850))
      deltaHrxn(T=298K) = -21.43832827189916 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4975000e+00 -9.7679000e-04 -8.2131000e-04 /
CHEB / 1.2021000e+01 3.2272000e-05 3.0088000e-05 /
CHEB / 6.1302000e-01 1.2071000e-03 1.0134000e-03 /
CHEB / 2.3476000e-01 3.1689000e-04 2.6191000e-04 /
CHEB / 9.6121000e-02 -3.7394000e-04 -3.1502000e-04 /
```

```
tSPC(1286)+HCO(+m)=tSPC(1416)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #304 (C4H4O4JJ(2850))    deltaHrxn(T=298K) = -
83.04173985394826 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2357000e+00 -4.9255000e-04 -3.4286000e-04 /
CHEB / 2.5675000e+00 -3.1006000e-05 -2.1582000e-05 /
CHEB / 1.0363000e+00 3.0525000e-04 2.1249000e-04 /
CHEB / 3.7094000e-01 1.6242000e-04 1.1306000e-04 /
CHEB / 1.1725000e-01 1.3763000e-05 9.5770000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+HCO(+m)=sSPC(3071)+tSPC(346)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #589 (C4H4O4(3244))
      deltaHrxn(T=298K) = -10.338700297674517 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1385000e+00 -7.6017000e-05 -5.2906000e-05 /
CHEB / 3.7580000e+00 -1.1490000e-04 -7.9965000e-05 /
CHEB / 1.1346000e+00 -9.1865000e-05 -6.3932000e-05 /
CHEB / 3.1122000e-01 -7.3864000e-05 -5.1404000e-05 /
CHEB / 7.9084000e-02 -5.2825000e-05 -3.6761000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+C2H3(+m)=HCO+CH2CHO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
16.628569545105595 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3116000e+01 -9.3866000e-02 -5.9916000e-02 /
CHEB / -4.6478000e-01 9.2742000e-02 5.8916000e-02 /
CHEB / 2.8229000e-03 2.1602000e-02 1.3523000e-02 /
CHEB / -1.5658000e-03 -1.7308000e-02 -1.0333000e-02 /
CHEB / -5.1485000e-04 -7.5985000e-03 -4.7404000e-03 /

HCO+CH2CHO(+m)=CO+C2H4O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
72.71265595603599 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1642000e+01 -6.2300000e-01 -2.2314000e-01 /
CHEB / 4.2269000e-01 6.0574000e-01 1.8014000e-01 /
CHEB / 1.2717000e-01 1.0818000e-01 6.9709000e-02 /
CHEB / -1.7598000e-02 -5.4010000e-02 -3.8120000e-03 /
CHEB / -1.0998000e-02 -4.1996000e-02 -1.8985000e-02 /

sSPC(2810)+C2H3(+m)=CO+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
89.34122550114158 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1213000e+01 -1.0310000e-01 -6.5686000e-02 /
CHEB / 5.6952000e-01 9.2131000e-02 5.8440000e-02 /
CHEB / 1.3017000e-01 3.2213000e-02 2.0018000e-02 /
CHEB / 4.8707000e-02 -1.4395000e-02 -8.4355000e-03 /
CHEB / 2.5005000e-02 -1.1028000e-02 -6.6953000e-03 /

HCO+CH2CHO(+m)=CO2+C2H4(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
98.20972123796768 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2805000e+01 -6.2809000e-01 -2.2473000e-01 /
CHEB / -5.7559000e-01 6.0444000e-01 1.7895000e-01 /
CHEB / -1.5120000e-01 1.1337000e-01 7.1071000e-02 /
CHEB / -1.1411000e-01 -5.1512000e-02 -2.3798000e-03 /
CHEB / -4.9922000e-02 -4.2720000e-02 -1.8672000e-02 /
```

```
sSPC(2810)+C2H3(+m)=CO2+C2H4(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
114.83829078307328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2288000e+01 -1.0381000e-01 -6.6131000e-02 /
CHEB / -3.8160000e-01 9.1949000e-02 5.8317000e-02 /
CHEB / -1.3495000e-01 3.2981000e-02 2.0488000e-02 /
CHEB / -4.5898000e-02 -1.4048000e-02 -8.2133000e-03 /
CHEB / -1.2307000e-02 -1.1217000e-02 -6.7989000e-03 /

CO+C2H4O(+m)=CO2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #843 (C3H4O2(1305))     deltaHrxn(T=298K) = -
25.497065281931704 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3268000e+01 -1.2400000e+00 -1.0439000e-01 /
CHEB / 2.0538000e+01 1.0174000e+00 -3.9561000e-02 /
CHEB / 4.1191000e-01 3.2682000e-01 9.0842000e-02 /
CHEB / -5.8341000e-02 -1.0090000e-02 6.4586000e-02 /
CHEB / -3.6450000e-02 -7.2272000e-02 6.2838000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(1553)+H(+m)=OH+C3H3O-enone(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #970 (C3H4O2(2841))     deltaHrxn(T=298K) = -
1.3799993405630353 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0073000e+01 -9.6001000e-01 -1.8318000e-01 /
CHEB / 1.8850000e+00 9.0966000e-01 8.1073000e-02 /
CHEB / 3.0820000e-01 1.7757000e-01 1.1771000e-01 /
CHEB / -8.5941000e-02 -4.6357000e-02 2.7197000e-02 /
CHEB / -3.1710000e-02 -5.9333000e-02 -2.0877000e-02 /
```

```
OH+C3H3O-enone(+m)=CO2+C2H4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #970 (C3H4O2(2841))     deltaHrxn(T=298K) = -
101.41903503144962 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1502000e+01 -1.1396000e+00 -1.5990000e-01 /
CHEB / 8.0903000e-01 9.2786000e-01 2.1299000e-02 /
CHEB / 3.4132000e-02 3.1328000e-01 1.0152000e-01 /
CHEB / -1.1738000e-01 4.4354000e-03 6.2049000e-02 /
CHEB / -1.0025000e-01 -6.3245000e-02 4.4171000e-03 /

tSPC(1553)+H(+m)=CO2+C2H4(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #970 (C3H4O2(2841))     deltaHrxn(T=298K) = -
102.79903437201267 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2155000e+01 -1.0891000e+00 -1.7486000e-01 /
CHEB / 2.7910000e-01 9.0314000e-01 4.3305000e-02 /
CHEB / 2.9844000e-02 2.9056000e-01 1.0456000e-01 /
CHEB / -9.3244000e-02 -3.2827000e-03 5.5745000e-02 /
CHEB / -7.6316000e-02 -6.2380000e-02 -6.3535000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     nSPC(543)   -19.98      81.66 17.04 21.8  24.57 26.89 30.56 33.29
      35.75 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

nSPC(543)+HCO(+m)=sSPC(3071)+CH2CHO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1105 (C3H4O4(3241))     deltaHrxn(T=298K) = -
9.519142418854791 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4918000e+00 -7.8339000e-03 -5.4245000e-03 /
CHEB / 2.3022000e+00 4.8213000e-03 3.3333000e-03 /
CHEB / 6.6231000e-01 1.3135000e-03 9.0688000e-04 /
CHEB / 1.7979000e-01 -1.4224000e-03 -9.8094000e-04 /
CHEB / 2.3858000e-02 -8.8728000e-04 -6.1331000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     sSPC(3071)  -24.8 66.19 14.25 16.54 18.3  19.62 21.42 22.5  23.78
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     tSPC(1286)  -14.81      85.93 22.22 26.75 30.07 32.59 36.26 38.87
      42.48 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

sSPC(3071)+C2H3(+m)=O2+C3H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C3H4O3JJ(337))      deltaHrxn(T=298K) = -
60.91379626671357 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4924000e+00 3.8937000e-11 2.7102000e-11 /
CHEB / 2.5738000e+00 7.6374000e-11 5.3165000e-11 /
CHEB / 1.8224000e-01 7.1944000e-11 5.0076000e-11 /
CHEB / 7.2979000e-02 6.4742000e-11 4.5067000e-11 /
CHEB / 3.0199000e-02 5.5057000e-11 3.8323000e-11 /

tSPC(1286)+H(+m)=O2+C3H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C3H4O3JJ(337))      deltaHrxn(T=298K) = -
50.8044424307615 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6452000e+00 2.8805000e-11 2.0049000e-11 /
CHEB / 3.6120000e+00 5.6500000e-11 3.9331000e-11 /
CHEB / 8.3950000e-03 5.3223000e-11 3.7045000e-11 /
CHEB / 2.0725000e-02 4.7896000e-11 3.3341000e-11 /
CHEB / 1.3229000e-02 4.0732000e-11 2.8351000e-11 /

tSPC(1286)+H(+m)=sSPC(3071)+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5 (C3H4O3JJ(337)) deltaHrxn(T=298K) =
10.10935383595207 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2078000e+01 -2.2486000e-09 -1.5652000e-09 /
CHEB / 1.9943000e+01 -4.3776000e-09 -3.0471000e-09 /
CHEB / 6.2450000e-01 -4.0343000e-09 -2.8082000e-09 /
CHEB / 1.9277000e-01 -3.5107000e-09 -2.4437000e-09 /
CHEB / 6.9355000e-02 -2.8654000e-09 -1.9945000e-09 /
```

```
tSPC(346)+HO2(+m)=O2+C3H4O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C3H4O3JJ(337))      deltaHrxn(T=298K) = -
63.03354957036987 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5344000e+00 4.2768000e-11 2.9768000e-11 /
CHEB / 3.1674000e+00 8.3922000e-11 5.8419000e-11 /
CHEB / 2.9227000e-01 7.9146000e-11 5.5090000e-11 /
CHEB / 1.0575000e-01 7.1349000e-11 4.9666000e-11 /
CHEB / 3.7544000e-02 6.0801000e-11 4.2321000e-11 /

sSPC(3071)+C2H3(+m)=tSPC(346)+HO2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5 (C3H4O3JJ(337)) deltaHrxn(T=298K) =
2.119753303656303 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1135000e+01 -2.7677000e-09 -1.9266000e-09 /
CHEB / 1.8718000e+01 -5.3899000e-09 -3.7518000e-09 /
CHEB / 9.4623000e-01 -4.9719000e-09 -3.4608000e-09 /
CHEB / 2.9099000e-01 -4.3331000e-09 -3.0161000e-09 /
CHEB / 1.0024000e-01 -3.5432000e-09 -2.4664000e-09 /

tSPC(1286)+H(+m)=tSPC(346)+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C3H4O3JJ(337))      deltaHrxn(T=298K) =
12.229107139608374 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5102000e+01 -2.3609000e-09 -1.6434000e-09 /
CHEB / 2.0938000e+01 -4.5969000e-09 -3.1998000e-09 /
CHEB / 6.7249000e-01 -4.2383000e-09 -2.9502000e-09 /
CHEB / 2.1774000e-01 -3.6909000e-09 -2.5691000e-09 /
CHEB / 7.9321000e-02 -3.0152000e-09 -2.0988000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
```

```
C2H3+sSPC(3071)(+m)=CH2CHO+sSPC(2810)(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1431 (C3H4O3(842))      deltaHrxn(T=298K) = -
78.23198116858798 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2651000e+01 -3.1391000e-05 -2.1849000e-05 /
CHEB / -3.4833000e-03 -4.7827000e-05 -3.3289000e-05 /
CHEB / -2.7258000e-02 -3.6619000e-05 -2.5487000e-05 /
CHEB / 1.3436000e-03 -3.0105000e-05 -2.0953000e-05 /
CHEB / -5.5529000e-03 -2.3794000e-05 -1.6561000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3C[OH]CH3 -23.1 75.32 21.79 26.16 30.18 33.31 38.7  42.75 49.39
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

CH3C[OH]CH3+OH(+m)=H2CCCH3[OH]+H2O(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C3H8O2(348))   deltaHrxn(T=298K) = -
82.82143594985979 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1885000e+01 -9.4968000e-01 -1.7196000e-01 /
CHEB / 7.6825000e-01 9.5334000e-01 8.7430000e-02 /
CHEB / -1.1998000e-02 1.6696000e-01 1.1738000e-01 /
CHEB / -9.5481000e-02 -9.2983000e-02 1.7336000e-02 /
CHEB / -5.6493000e-02 -8.3771000e-02 -3.3527000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
```

```
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+C4H7-24=sSPC(56)     2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+pC3H5=sSPC(56)      1.4157154e+13      -0.15000
2.9166667e+02
!     sSPC(56)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04

O2+C4H7-24(+m)=sSPC(56)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56)) High-P Limit: R_Recombination estimate:
(Average:) O2_birad     C_rad/H2/Cd       deltaHrxn(T=298K) = -
20.837910544011862 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8323000e+00 1.1962000e+00 -1.4471000e-01 /
CHEB / -6.0669000e+00 9.0165000e-01 1.4165000e-01 /
CHEB / -3.1500000e+00 1.1742000e-01 4.1554000e-02 /
CHEB / -1.3874000e+00 -1.7073000e-01 -2.4527000e-02 /
CHEB / -4.3854000e-01 -1.0059000e-01 -3.1256000e-02 /

nSPC(102)+pC3H5(+m)=sSPC(56)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/O     Cd_pri_rad      deltaHrxn(T=298K) = -
101.98948851758314 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6291000e+01 7.5372000e+00 1.6615000e+00 /
CHEB / -6.2003000e+00 2.2209000e-01 1.1972000e-01 /
CHEB / -3.3381000e+00 -2.4056000e-01 -2.3538000e-02 /
CHEB / -1.3781000e+00 -2.1505000e-01 -4.2468000e-02 /
CHEB / -4.1415000e-01 -8.3778000e-02 -3.0149000e-02 /

nSPC(102)+pC3H5(+m)=O2+C4H7-24(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56))     deltaHrxn(T=298K) = -81.15157797357128
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3447000e+01 1.6895000e-06 1.1761000e-06 /
CHEB / -7.4707000e-01 1.8230000e-06 1.2690000e-06 /
CHEB / -7.6273000e-02 4.5618000e-07 3.1748000e-07 /
CHEB / -3.1914000e-02 -1.2718000e-07 -8.8558000e-08 /
CHEB / -2.5909000e-02 -2.3997000e-07 -1.6704000e-07 /
```

```
HO2+C4H6-12(+m)=sSPC(56)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56))     deltaHrxn(T=298K) = -29.416988159461347
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5908000e+00 3.4191000e+00 -3.1181000e-01 /
CHEB / -5.2604000e+00 3.8866000e-01 2.6962000e-01 /
CHEB / -3.0080000e+00 -4.0227000e-02 7.3157000e-02 /
CHEB / -1.2858000e+00 -1.8887000e-01 -3.3235000e-02 /
CHEB / -3.8554000e-01 -9.6869000e-02 -3.5726000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(1151)  -40.72      90.25 26.29 31.91 36.7  40.82 47.76 52.72
      57.44 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     OCH2CH2CH3  -9.17 75.06 20.0  24.84 29.16 32.91 38.84 43.25 48.01
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH3C[O]CH2cH2     -7.88 84.48 23.4  28.34 32.68 36.44 42.87 47.61
      54.18 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!Here are the path reactions and their high-P limit kinetics:
!     CH2O+CH2C[O]CH3=sSPC(1151)    7.9400000e+10      0.00000
6.7000000e+03
!     OCH2CH2CH3+CO=sSPC(1151)      5.3800000e+02      3.29000
1.0450000e+05
!     O+CH3C[O]CH2cH2=sSPC(1151)    1.0000000e+13      0.00000
0.0000000e+00

C4H6O(717)+OH(+m)=sSPC(1151)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (C4H7O2J(394))      deltaHrxn(T=298K) = -
19.637811606084277 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -6.5804000e+00 5.3603000e+00 -6.9003000e-02 /
CHEB / 2.5173000e+00 6.7310000e-02 3.1620000e-01 /
CHEB / -2.5459000e+00 -3.4204000e-01 1.2122000e-01 /
CHEB / -1.1907000e+00 -2.3919000e-01 -4.9593000e-02 /
CHEB / -4.4105000e-01 -2.7074000e-03 -8.8067000e-02 /

CH2O+CH2C[O]CH3(+m)=sSPC(1151)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (C4H7O2J(394)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H2_O     C_rad/H2/CO          deltaHrxn(T=298K)
= -11.858773913629754 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5423000e+00 1.3056000e+00 -1.3602000e-01 /
CHEB / -3.8369000e+00 8.0134000e-01 1.4739000e-01 /
CHEB / -2.9943000e+00 5.9063000e-02 2.0667000e-02 /
CHEB / -1.2598000e+00 -1.6107000e-01 -1.9844000e-02 /
CHEB / -3.8530000e-01 -6.6614000e-02 -2.3617000e-02 /

C4H6O(717)+OH(+m)=CH2O+CH2C[O]CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #73 (C4H7O2J(394)) deltaHrxn(T=298K) = -
7.779037692454522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6557000e+00 -3.6203000e-01 -1.8163000e-01 /
CHEB / 6.6707000e+00 4.3919000e-01 2.0449000e-01 /
CHEB / 3.8623000e-02 -1.6057000e-02 1.6196000e-02 /
CHEB / -8.4339000e-02 -6.1960000e-02 -3.3416000e-02 /
CHEB / -7.7072000e-02 -1.7029000e-02 -1.6213000e-02 /

sSPC(1151)(+m)=OCH2CH2CH3+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (C4H7O2J(394))      deltaHrxn(T=298K) =
5.129342971288835 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7475000e+01 1.0320000e+01 3.9179000e+00 /
CHEB / 3.4697000e+01 3.6248000e-01 -7.0465000e-01 /
CHEB / -1.6382000e+00 -9.9995000e-02 -7.0618000e-01 /
CHEB / -6.6351000e-01 4.3710000e-02 -3.5364000e-01 /
CHEB / -2.5837000e-01 1.2142000e-01 -5.9268000e-02 /

C4H6O(717)+OH(+m)=OCH2CH2CH3+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (C4H7O2J(394))      deltaHrxn(T=298K) = -
14.508468634795443 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.7390000e+01 6.3771000e-04 4.4659000e-04 /
CHEB / 3.3060000e+01 -7.5028000e-04 -5.2600000e-04 /
CHEB / 5.1560000e-01 6.9981000e-05 4.9716000e-05 /
CHEB / 7.9665000e-02 5.8312000e-05 4.0698000e-05 /
CHEB / -3.8010000e-02 1.3002000e-05 9.0080000e-06 /

CH2O+CH2C[O]CH3(+m)=OCH2CH2CH3+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #73 (C4H7O2J(394)) deltaHrxn(T=298K) = -
6.729430942340919 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / -2.8346000e+01 7.7399000e-06 5.3872000e-06 /
CHEB / 3.4386000e+01 1.2644000e-05 8.8008000e-06 /
CHEB / 2.5795000e-01 6.2733000e-06 4.3668000e-06 /
CHEB / 1.4470000e-02 -1.9809000e-08 -1.3370000e-08 /
CHEB / -4.5948000e-02 -3.9970000e-06 -2.7818000e-06 /

O+CH3C[O]CH2cH2(+m)=sSPC(1151)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #73 (C4H7O2J(394)) High-P Limit: Oa_R_Recombination
estimate: (Average:) Oa     C_rad/H2/Cs         deltaHrxn(T=298K) = -
92.38045357102577 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6535000e+01 9.1506000e+00 2.9754000e+00 /
CHEB / -3.5345000e+00 1.0382000e+00 -5.6313000e-01 /
CHEB / -1.7518000e+00 -1.0979000e-01 -6.3927000e-01 /
CHEB / -8.7678000e-01 -1.9015000e-01 -2.2501000e-01 /
CHEB / -4.4535000e-01 -9.4358000e-02 5.9855000e-02 /

O+CH3C[O]CH2cH2(+m)=C4H6O(717)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #73 (C4H7O2J(394)) deltaHrxn(T=298K) = -
72.74264196494148 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1101000e+01 1.3445000e-03 9.3547000e-04 /
CHEB / 7.0389000e-01 -1.6472000e-03 -1.1421000e-03 /
CHEB / 3.1309000e-01 1.6042000e-04 1.0345000e-04 /
CHEB / 1.2064000e-02 1.6299000e-04 1.1849000e-04 /
CHEB / -6.9215000e-02 2.3095000e-05 1.5701000e-05 /

O+CH3C[O]CH2cH2(+m)=CH2O+CH2C[O]CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #73 (C4H7O2J(394)) deltaHrxn(T=298K) = -
80.52167965739602 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4003000e+01 5.8369000e-06 4.0628000e-06 /
CHEB / -1.0879000e+00 1.0576000e-05 7.3616000e-06 /
CHEB / -1.6731000e-01 6.6122000e-06 4.6026000e-06 /
CHEB / -1.3024000e-01 2.0813000e-06 1.4488000e-06 /
CHEB / -1.0526000e-01 -1.2630000e-06 -8.7895000e-07 /

O+CH3C[O]CH2cH2(+m)=OCH2CH2CH3+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #73 (C4H7O2J(394)) deltaHrxn(T=298K) = -
87.25111059973693 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1194000e+00 -3.9183000e-04 -2.7269000e-04 /
CHEB / 9.6252000e+00 1.8827000e-04 1.3103000e-04 /
CHEB / 1.1852000e+00 2.0605000e-04 1.4339000e-04 /
CHEB / 3.0660000e-01 4.8088000e-05 3.3469000e-05 /
CHEB / 2.6586000e-02 -1.9011000e-05 -1.3223000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+CH2O(+m)=tSPC(54)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #126 (C4H7O2J(717))     deltaHrxn(T=298K) =
42.89562258098408 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1053000e+01 -1.9892000e-14 -1.3148000e-14 /
CHEB / 2.5022000e+01 1.1288000e-12 7.8407000e-13 /
CHEB / -1.1616000e-01 3.5051000e-12 2.4429000e-12 /
CHEB / 2.0984000e-01 4.8367000e-12 3.3620000e-12 /
CHEB / 1.2240000e-01 3.8325000e-12 2.6740000e-12 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     MEKenol     -46.68      81.2  24.43 29.77 34.47 38.61 45.55 50.67
      58.38 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH3C[O]cHCH3      -10.78      80.09 23.09 27.78 31.99 35.82 42.42
      47.34 54.59 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

MEKenol+O(+m)=CH3C[O]cHCH3+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #198 (C4H8O2JJ(733))    deltaHrxn(T=298K) = -
14.328714807706012 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5499000e+00 -6.8530000e-05 -4.7693000e-05 /
CHEB / 3.7468000e+00 -1.3153000e-04 -9.1537000e-05 /
CHEB / 2.5611000e-01 -1.1674000e-04 -8.1245000e-05 /
CHEB / 7.1687000e-02 -9.6524000e-05 -6.7172000e-05 /
CHEB / 1.0510000e-02 -7.4579000e-05 -5.1900000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

nSPC(801)+O(+m)=sSPC(1909)+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #223 (C2H3O4JJJ(1026))  deltaHrxn(T=298K) = -
25.797063920922863 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0411000e+01 -1.6263000e-04 -1.1314000e-04 /
CHEB / 1.4937000e+00 -3.1541000e-04 -2.1944000e-04 /
CHEB / -6.5084000e-02 -2.8750000e-04 -2.0002000e-04 /
CHEB / -7.3839000e-02 -2.4586000e-04 -1.7104000e-04 /
CHEB / -6.6317000e-02 -1.9624000e-04 -1.3652000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+O(+m)=sSPC(1909)+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #288 (C3H5O2JJJ(880))   deltaHrxn(T=298K) = -
24.207637486317985 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0850000e+01 -1.1388000e-08 -7.9272000e-09 /
CHEB / 1.1588000e+00 1.6058000e-08 1.1178000e-08 /
CHEB / -3.8029000e-02 3.1938000e-08 2.2231000e-08 /
CHEB / -3.3617000e-02 3.6253000e-09 2.5235000e-09 /
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CHEB / -2.9156000e-02 -1.1467000e-08 -7.9818000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     sSPC(3071)  -24.8 66.19 14.25 16.54 18.3  19.62 21.42 22.5  23.78
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CO2               -94.36      50.99 8.87  9.84  10.63 11.26 12.23
      12.9  13.82
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     sSPC(2810)  -29.51      59.94 9.81  11.32 12.68 13.78 15.39 16.47
      17.98
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     OH+CO2=OCOOH            2.3501400e+11      0.30815
4.9629937e+03
!     sSPC(3071)=OCOOH        2.0320555e+08      1.13906
3.4790987e+04
!     O2+HCO=sSPC(3071)       3.5000000e+12      0.00000
0.0000000e+00
!     HO2+CO=sSPC(3071)       5.9198482e+04      2.36750
7.2970000e+04
!     sSPC(2810)+O=sSPC(3071) 1.0000000e+13      0.00000
0.0000000e+00
!     HO2+CO=OCOOH            3.4100000e+07      0.00000
3.0000000e+03

sSPC(3071)(+m)=OCOOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH) High-P Limit: intra_H_migration estimate:
(Average:) Others-R3H_SS    O_rad_out     CO_H_out
      deltaHrxn(T=298K) = 0.06968666240125287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8123000e+01 2.8330000e+00 -3.8376000e-01 /
CHEB / 2.9263000e+01 4.8254000e-01 -9.5007000e-02 /
CHEB / -8.8684000e-01 1.8509000e-01 -1.3727000e-02 /
CHEB / -4.3347000e-01 6.1522000e-02 -7.1263000e-04 /
CHEB / -1.9019000e-01 1.2413000e-02 1.3221000e-03 /

OCOOH(+m)=OH+CO2(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = -60.93382374602254 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7179000e+00 2.0000000e+00 -3.1266000e-08 /
CHEB / 2.1742000e+00 -8.8095000e-08 -6.1321000e-08 /
CHEB / -8.0809000e-01 -8.2943000e-08 -5.7735000e-08 /
CHEB / -3.3111000e-01 -7.4592000e-08 -5.1922000e-08 /
CHEB / -1.2366000e-01 -6.3380000e-08 -4.4117000e-08 /

sSPC(3071)(+m)=OH+CO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = -60.86413708362129 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0740000e+00 9.8013000e-01 -3.2258000e-01 /
CHEB / 1.0198000e+01 7.0709000e-01 -8.9730000e-03 /
CHEB / -8.8280000e-01 3.0001000e-01 2.0749000e-02 /
CHEB / -4.2648000e-01 1.0524000e-01 6.0301000e-03 /
CHEB / -1.8907000e-01 2.5713000e-02 1.8672000e-04 /

O2+HCO(+m)=OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = -35.4865240684176 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6062000e+01 2.0524000e+00 -1.1519000e-01 /
CHEB / 1.9232000e+01 2.7368000e-02 1.9965000e-02 /
CHEB / -2.7727000e-01 3.8554000e-02 3.5204000e-02 /
CHEB / -1.4928000e-01 1.9726000e-02 1.7367000e-02 /
CHEB / -6.6371000e-02 4.8985000e-03 5.4598000e-03 /

O2+HCO(+m)=sSPC(3071)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH) High-P Limit: R_Recombination exact:  O2_birad
CO_pri_rad        deltaHrxn(T=298K) = -35.556210730818854 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3446000e+00 2.5229000e+00 -3.9020000e-01 /
CHEB / -1.4389000e+00 2.6581000e-01 -8.7940000e-02 /
CHEB / -9.1481000e-01 1.1843000e-01 1.1561000e-02 /
CHEB / -4.2594000e-01 4.1839000e-02 1.7310000e-02 /
CHEB / -1.9118000e-01 5.7336000e-03 1.0163000e-02 /

O2+HCO(+m)=OH+CO2(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = -96.42034781444015 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1774000e+00 -2.8896000e-02 -4.0729000e-02 /
CHEB / 1.2073000e+00 1.8559000e-02 3.4863000e-02 /
CHEB / 2.8925000e-01 1.6871000e-02 1.3834000e-02 /
CHEB / 1.2352000e-01 -1.3850000e-03 -3.6892000e-03 /
CHEB / 5.5936000e-02 -4.2597000e-03 -4.0516000e-03 /

OCOOH(+m)=HO2+CO(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = 1.3599737868545851 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0853000e+01 2.0000000e+00 -8.6962000e-09 /
CHEB / 2.0701000e+01 -2.4499000e-08 -1.7053000e-08 /
CHEB / -8.9931000e-01 -2.3056000e-08 -1.6049000e-08 /
CHEB / -3.6344000e-01 -2.0722000e-08 -1.4424000e-08 /
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CHEB / -1.3676000e-01 -1.7595000e-08 -1.2247000e-08 /

sSPC(3071)(+m)=HO2+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = 1.429660449255838 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0164000e+01 9.8626000e-01 -3.2016000e-01 /
CHEB / 2.8711000e+01 7.1615000e-01 -5.8067000e-03 /
CHEB / -9.7942000e-01 3.0433000e-01 2.1790000e-02 /
CHEB / -4.6021000e-01 1.0660000e-01 6.0081000e-03 /
CHEB / -2.0241000e-01 2.6034000e-02 2.5160000e-05 /

!HO2+CO(+m)=OH+CO2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = -62.29379753287713 kcal/mol
!TCHEB / 290.0 3000.0 / PCHEB / 0.009869232667160128 98.69232667160128 /
!CHEB / 5   3 /
!CHEB / 5.2023000e+00 1.2289000e-09 8.5548000e-10 /
!CHEB / 2.4790000e+00 2.4122000e-09 1.6793000e-09 /
!CHEB / -3.1265000e-01 2.2769000e-09 1.5851000e-09 /
!CHEB / -1.0667000e-01 2.0554000e-09 1.4309000e-09 /
!CHEB / -2.8941000e-02 1.7542000e-09 1.2212000e-09 /

O2+HCO(+m)=HO2+CO(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (OCOOH)  deltaHrxn(T=298K) = -34.12655028156302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.0051000e+00 2.3170000e-07 1.6128000e-07 /
CHEB / 1.4042000e+01 3.1538000e-07 2.1953000e-07 /
CHEB / 2.4670000e-01 1.5635000e-07 1.0883000e-07 /
CHEB / 9.5538000e-02 6.3919000e-08 4.4492000e-08 /
CHEB / 3.1028000e-02 2.3975000e-08 1.6689000e-08 /

sSPC(2810)+O(+m)=OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = -54.85468647033519 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1878000e+01 2.1469000e+00 1.0151000e-01 /
CHEB / 1.9223000e+01 2.2687000e-01 1.5420000e-01 /
CHEB / -1.9146000e-01 1.3360000e-01 8.7112000e-02 /
CHEB / -1.2457000e-01 5.9323000e-02 3.5624000e-02 /
CHEB / -5.6208000e-02 1.8273000e-02 8.9639000e-03 /

sSPC(2810)+O(+m)=sSPC(3071)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/OneDe     Oa       deltaHrxn(T=298K) = -
54.92437313273644 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2895000e-01 4.8508000e+00 -1.4351000e-02 /
CHEB / 2.4898000e-01 -1.9570000e-01 7.3600000e-02 /
CHEB / -1.5968000e-01 -3.7140000e-01 6.7179000e-02 /
CHEB / -2.8143000e-01 -1.3539000e-01 6.7613000e-02 /
CHEB / -3.3382000e-01 9.7991000e-02 3.7431000e-02 /

sSPC(2810)+O(+m)=OH+CO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = -115.78851021635774 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 9.5558000e+00 2.2573000e-05 1.5720000e-05 /
CHEB / 1.1677000e+00 -4.4522000e-06 -3.0968000e-06 /
CHEB / 3.6017000e-01 -1.1275000e-05 -7.8530000e-06 /
CHEB / 1.2668000e-01 -3.7858000e-06 -2.6385000e-06 /
CHEB / 4.6366000e-02 4.2702000e-07 2.9659000e-07 /

sSPC(2810)+O(+m)=O2+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = -19.368162401917587 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3344000e+01 1.3968000e-07 9.6999000e-08 /
CHEB / -2.9853000e-01 3.1788000e-07 2.2108000e-07 /
CHEB / -1.2825000e-02 2.0286000e-07 1.4133000e-07 /
CHEB / -4.1957000e-03 6.4194000e-08 4.4883000e-08 /
CHEB / -6.2718000e-03 -1.0913000e-08 -7.4867000e-09 /

sSPC(2810)+O(+m)=HO2+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (OCOOH)  deltaHrxn(T=298K) = -53.4947126834806 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8871000e+00 -9.9859000e-06 -6.9510000e-06 /
CHEB / 7.9699000e+00 1.1632000e-09 7.9188000e-10 /
CHEB / 3.9634000e-01 4.2545000e-06 2.9615000e-06 /
CHEB / 1.3635000e-01 2.1561000e-06 1.5009000e-06 /
CHEB / 4.2608000e-02 4.5275000e-07 3.1515000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     nSPC(801)   -35.7 78.62 20.26 23.92 26.85 29.15 32.42 34.49 37.2
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2+sSPC(3121)(+m)=CH2CHO+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #392 (C2H4O3JJ(985))    deltaHrxn(T=298K) = -
13.998142739287355 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0270000e+01 -6.1481000e-05 -4.2793000e-05 /
```

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CHEB / 6.9187000e-01 -4.0534000e-05 -2.8211000e-05 /
CHEB / -3.7365000e-01 -7.4296000e-06 -5.1702000e-06 /
CHEB / -1.3031000e-01 -6.2877000e-06 -4.3761000e-06 /
CHEB / -2.4507000e-02 -5.2516000e-06 -3.6554000e-06 /

nSPC(801)+H(+m)=CH2+sSPC(3121)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #392 (C2H4O3JJ(985))    deltaHrxn(T=298K) =
7.419395498127116 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0442000e+01 -6.1481000e-05 -4.2793000e-05 /
CHEB / 3.0153000e+00 -4.0534000e-05 -2.8211000e-05 /
CHEB / -2.7548000e-01 -7.4296000e-06 -5.1702000e-06 /
CHEB / -8.6756000e-02 -6.2877000e-06 -4.3761000e-06 /
CHEB / -6.2079000e-03 -5.2516000e-06 -3.6554000e-06 /

nSPC(801)+H(+m)=CH2CHO+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #392 (C2H4O3JJ(985))    deltaHrxn(T=298K) = -
6.57874724116023 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2127000e+01 -8.7139000e-05 -6.0649000e-05 /
CHEB / -1.1373000e-01 -7.6618000e-05 -5.3321000e-05 /
CHEB / -4.3392000e-01 -1.6219000e-05 -1.1283000e-05 /
CHEB / -1.9590000e-01 3.0330000e-06 2.1127000e-06 /
CHEB / -6.4396000e-02 9.3782000e-06 6.5262000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHO            6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     sSPC(1909)  -2.38 66.97 14.01 16.31 18.37 20.02 22.65 24.45 25.52
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHO+O(+m)=sSPC(2810)+CH2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #475 (C2H3O2JJJ(341))   deltaHrxn(T=298K) = -
11.798921208496083 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0198000e+01 -1.2482000e-06 -8.6910000e-07 /
CHEB / 1.7314000e+00 5.5614000e-08 3.8900000e-08 /
CHEB / 2.2041000e-03 8.0755000e-07 5.6229000e-07 /
CHEB / -6.3047000e-03 3.4552000e-07 2.4048000e-07 /
CHEB / -1.1529000e-02 -1.5517000e-08 -1.0854000e-08 /
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sSPC(1909)+H(+m)=CH2CHO+O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #475 (C2H3O2JJJ(341))   deltaHrxn(T=298K) =
19.218316679762637 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2208000e-01 -9.4519000e-06 -6.5795000e-06 /
CHEB / 7.9943000e+00 6.2143000e-06 4.3258000e-06 /
CHEB / 2.0544000e-01 3.9357000e-06 2.7397000e-06 /
CHEB / 1.1109000e-01 -1.4902000e-07 -1.0377000e-07 /
CHEB / 5.3239000e-02 -7.1769000e-07 -4.9962000e-07 /

sSPC(1909)+H(+m)=sSPC(2810)+CH2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #475 (C2H3O2JJJ(341))   deltaHrxn(T=298K) =
7.419395471266554 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.9561000e+00 -1.2837000e-04 -8.9346000e-05 /
CHEB / 4.2846000e+00 1.2316000e-04 8.5718000e-05 /
CHEB / -1.0039000e-01 3.9442000e-05 2.7447000e-05 /
CHEB / 5.2227000e-02 -2.5806000e-05 -1.7959000e-05 /
CHEB / 3.9027000e-02 -1.5545000e-05 -1.0817000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     tSPC(122)   -4.22 107.47      35.61 41.91 47.13 51.65 58.53 64.16
      71.73 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

tSPC(54)+HO2(+m)=O2+C4H8O2(62)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O4JJ(334))      deltaHrxn(T=298K) = -
38.48624278252174 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3490000e+00 1.3473000e-10 9.3782000e-11 /
CHEB / 3.7875000e+00 2.6425000e-10 1.8394000e-10 /
CHEB / -3.9136000e-02 2.4882000e-10 1.7320000e-10 /
CHEB / -2.0897000e-02 2.2380000e-10 1.5578000e-10 /
CHEB / -2.8939000e-02 1.9019000e-10 1.3239000e-10 /
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tSPC(122)+H(+m)=tSPC(54)+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O4JJ(334))      deltaHrxn(T=298K) = -
30.7661873923174 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8983000e-01 -1.0867000e-08 -7.5641000e-09 /
CHEB / 1.0134000e+01 -2.0456000e-08 -1.4239000e-08 /
CHEB / 3.2561000e-01 -1.6992000e-08 -1.1828000e-08 /
CHEB / 7.6703000e-02 -1.2295000e-08 -8.5579000e-09 /
CHEB / -1.2677000e-02 -7.5389000e-09 -5.2476000e-09 /

tSPC(122)+H(+m)=O2+C4H8O2(62)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H8O4JJ(334))      deltaHrxn(T=298K) = -
69.25243017483915 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3207000e+01 3.5563000e-10 2.4754000e-10 /
CHEB / 3.8228000e-01 6.9743000e-10 4.8547000e-10 /
CHEB / -2.5605000e-02 6.5657000e-10 4.5702000e-10 /
CHEB / -3.5321000e-03 5.9035000e-10 4.1093000e-10 /
CHEB / -1.4598000e-02 5.0151000e-10 3.4908000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

CH2OOH+C4H6Oi-13(+m)=C4H8O2(62)+HCO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) =
0.6699106382919204 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 6.7773000e+00 -1.1440000e-01 -6.8780000e-02 /
CHEB / 3.8543000e+00 1.6462000e-01 9.7057000e-02 /
CHEB / -4.2137000e-02 -4.9335000e-02 -2.5609000e-02 /
CHEB / -7.6734000e-02 -7.6954000e-03 -7.2487000e-03 /
CHEB / -6.2213000e-02 5.9562000e-03 3.7002000e-03 /

tSPC(213)+CH3(+m)=C4H8O2(62)+HCO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) = -
0.8696208413335782 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9655000e+00 -9.2223000e-02 -5.7223000e-02 /
CHEB / 3.8746000e+00 1.3324000e-01 8.1352000e-02 /
CHEB / -5.2966000e-02 -4.1098000e-02 -2.2684000e-02 /
CHEB / -5.0533000e-02 -4.9843000e-03 -4.9882000e-03 /
CHEB / -4.5103000e-02 4.4350000e-03 2.9254000e-03 /

tSPC(213)+CH3(+m)=CH2OOH+C4H6Oi-13(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) = -
1.5395314796254986 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4855000e+00 -8.7273000e-02 -5.4124000e-02 /
CHEB / 5.0904000e+00 1.2594000e-01 7.6926000e-02 /
CHEB / 1.9367000e-01 -3.8609000e-02 -2.1448000e-02 /
CHEB / 2.4838000e-02 -4.9510000e-03 -4.7071000e-03 /
CHEB / -2.2260000e-02 4.3441000e-03 2.8104000e-03 /

CH2OOH+tSPC(110)(+m)=C4H8O2(62)+HCO(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) = -
52.73468863968876 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3609000e+01 -1.7301000e-05 -1.2088000e-05 /
CHEB / -1.0763000e+00 5.6530000e-06 3.9597000e-06 /
CHEB / -1.6004000e-01 1.6478000e-05 1.1511000e-05 /
CHEB / -1.0865000e-01 2.6273000e-06 1.8213000e-06 /
CHEB / -8.3984000e-02 -4.8025000e-06 -3.3596000e-06 /

CH2OOH+tSPC(110)(+m)=CH2OOH+C4H6Oi-13(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) = -
53.40459927798068 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1545000e+01 -1.5066000e-04 -1.0505000e-04 /
CHEB / -2.5338000e-01 1.3378000e-04 9.3297000e-05 /
CHEB / 8.0126000e-02 5.0938000e-05 3.5519000e-05 /
CHEB / -2.6499000e-02 -1.7446000e-05 -1.2194000e-05 /
CHEB / -5.5234000e-02 -1.7150000e-05 -1.1961000e-05 /

CH2OOH+tSPC(110)(+m)=tSPC(213)+CH3(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #568 (C5H9O3J(1965))     deltaHrxn(T=298K) = -
51.86506779835518 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1858000e+01 -2.8117000e-04 -1.9598000e-04 /
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CHEB / -2.9890000e-01 2.6322000e-04 1.8350000e-04 /
CHEB / 9.1250000e-02 8.0452000e-05 5.6067000e-05 /
CHEB / -2.5736000e-02 -3.8541000e-05 -2.6905000e-05 /
CHEB / -5.8924000e-02 -2.8345000e-05 -1.9754000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH3+C3H3O-enone(+m)=C4H6O(717)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #827 (C4H6OJJ(427))     deltaHrxn(T=298K) = -
75.78164943989717 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9369000e+00 -5.1198000e-03 -3.5536000e-03 /
CHEB / 2.3723000e+00 3.4205000e-03 2.3695000e-03 /
CHEB / -4.1441000e-02 -7.1936000e-04 -4.9703000e-04 /
CHEB / 1.6587000e-02 -5.0091000e-04 -3.4776000e-04 /
CHEB / 9.7098000e-03 6.0825000e-05 4.1958000e-05 /

!PDepNetwork tSPC(110) && C4H6O(105) && C4H6Oi-13
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H6O(105)  -2.12 71.03 19.46 26.19 31.81 36.09 42.58 47.31 53.93
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H5OJ(14) 14.08 76.7  22.34 26.71 30.14 32.93 37.32 40.67 46.0
!MRH CBS-QB3 w/1DHR corrections
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     iC4H5OJ(15) 12.77 74.84 22.08 26.8  30.77 34.04 39.05 42.66 48.02
!MRH CBS-QB3 w/1DHR corrections
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
```

```
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!Here are the path reactions and their high-P limit kinetics:
!     tSPC(346)+CH3=tSPC(110) 1.5800000e+11      0.00000
4.9700000e+03
!     iC4H5OJ(14)+H=tSPC(110) 5.2263889e+12      0.04600
5.0666667e+03
!     iC4H5OJ(15)+H=tSPC(110) 1.0000000e+13      0.00000
1.2000000e+03
!     tSPC(110)=C4H6O(105)    5.8853831e+11      0.02483
1.8800000e+03
!     tSPC(110)=C4H6Oi-13     1.2640000e+08      0.00000
0.0000000e+00
!     sC3H5+HCO=C4H6Oi-13     1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(346)+CH3=C4H6Oi-13 1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H5OJ(14)+H=C4H6Oi-13 1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H5OJ(15)+H=C4H6Oi-13 5.0000000e+13      0.00000
0.0000000e+00
!     C3H6+CO=C4H6Oi-13       5.9198482e+04      2.36750
7.2970000e+04

tSPC(110)(+m)=C4H6O(105)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: Birad_recombination estimate:
(Average:) R4_SDS     O_rad     Cpri_rad_out_2H       deltaHrxn(T=298K)
= -28.186480807096594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2524000e+00 1.9919000e+00 -4.5079000e-02 /
CHEB / -3.4085000e+00 1.5664000e-01 3.2291000e-02 /
CHEB / -2.5458000e+00 3.5722000e-02 -1.2423000e-02 /
CHEB / -1.2961000e+00 -1.8653000e-02 -6.4366000e-03 /
CHEB / -6.6919000e-01 -6.5966000e-02 -5.8619000e-04 /

tSPC(110)(+m)=C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: 1,2-Birad_to_alkene exact:
Y_12_11           deltaHrxn(T=298K) = -53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0496000e+00 1.6266000e+00 -3.5830000e-02 /
CHEB / -1.9688000e+00 -3.9759000e-01 3.5329000e-02 /
CHEB / -1.5087000e+00 -1.8314000e-01 -6.5214000e-02 /
CHEB / -7.7196000e-01 6.0360000e-02 -8.0383000e-02 /
CHEB / -5.6327000e-01 1.4588000e-01 -2.8508000e-02 /

C4H6O(105)(+m)=C4H6Oi-13(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -25.218118470884093
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / -3.5913000e+00 2.4766000e-01 -5.9898000e-02 /
CHEB / 8.6009000e+00 5.8328000e-01 -2.0018000e-02 /
CHEB / -1.7001000e+00 3.6966000e-01 -4.3004000e-02 /
CHEB / -1.2202000e+00 2.0151000e-01 -5.1745000e-03 /
CHEB / -8.6718000e-01 3.7128000e-02 2.2209000e-02 /

tSPC(346)+CH3(+m)=tSPC(110)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Addition_MultipleBond exact:
Ca_Cd/H2     C_methyl         deltaHrxn(T=298K) = -55.62404666306642
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3869000e+00 8.2724000e-01 1.9480000e-03 /
CHEB / -1.1558000e+00 1.9574000e+00 -4.0741000e-01 /
CHEB / -1.8334000e+00 5.7057000e-01 -2.4567000e-02 /
CHEB / -1.2668000e+00 6.8145000e-02 1.1468000e-02 /
CHEB / -7.9189000e-01 -1.4047000e-01 -3.4711000e-02 /

tSPC(346)+CH3(+m)=C4H6O(105)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -83.81052747016302
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4058000e+00 7.2858000e-01 -6.2340000e-02 /
CHEB / -2.4161000e+00 2.0770000e+00 -3.3014000e-01 /
CHEB / -2.4765000e+00 5.6229000e-01 -2.8184000e-02 /
CHEB / -1.5413000e+00 5.7120000e-02 3.8345000e-03 /
CHEB / -8.7864000e-01 -1.4634000e-01 -3.8380000e-02 /

tSPC(346)+CH3(+m)=C4H6Oi-13(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/OneDe     C_methyl      deltaHrxn(T=298K) = -
109.02864594104712 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1384000e+01 1.1598000e+00 -2.7826000e-01 /
CHEB / -2.1901000e+00 1.5859000e+00 -2.0468000e-01 /
CHEB / -1.5031000e+00 8.4301000e-01 -2.9145000e-04 /
CHEB / -9.1156000e-01 3.4640000e-01 6.2978000e-02 /
CHEB / -5.4626000e-01 1.1546000e-01 4.6956000e-02 /

iC4H5OJ(14)+H(+m)=tSPC(110)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ck_O     H_rad       deltaHrxn(T=298K) = -
40.105398871178494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2110000e+00 9.5667000e-01 -3.2808000e-02 /
CHEB / -2.2010000e-01 1.3411000e+00 -2.0918000e-01 /
CHEB / -1.7256000e+00 7.6969000e-01 5.2635000e-02 /
CHEB / -1.2797000e+00 1.8519000e-01 1.2895000e-01 /
CHEB / -8.3308000e-01 -1.6858000e-01 1.1026000e-01 /

iC4H5OJ(14)+H(+m)=C4H6O(105)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -68.2918796782751
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2316000e+00 8.6028000e-01 -9.6715000e-02 /
CHEB / -1.4823000e+00 1.4585000e+00 -1.3194000e-01 /
CHEB / -2.3664000e+00 7.6438000e-01 4.9734000e-02 /
CHEB / -1.5544000e+00 1.7383000e-01 1.2136000e-01 /
CHEB / -9.1914000e-01 -1.7337000e-01 1.0703000e-01 /

iC4H5OJ(14)+H(+m)=C4H6Oi-13(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/OneDe     H_rad         deltaHrxn(T=298K) = -
93.50999814915919 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1992000e+01 5.1531000e-01 -6.7956000e-02 /
CHEB / -1.3619000e+00 9.1758000e-01 -1.0170000e-01 /
CHEB / -1.0928000e+00 6.5327000e-01 -3.2719000e-02 /
CHEB / -7.5599000e-01 3.7120000e-01 2.1504000e-02 /
CHEB / -4.9853000e-01 1.6422000e-01 3.9357000e-02 /

iC4H5OJ(14)+H(+m)=tSPC(346)+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 15.518647791887929
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3464000e+00 -1.1198000e+00 -1.2608000e-01 /
CHEB / 6.4179000e+00 1.0030000e+00 1.7361000e-02 /
CHEB / 1.0450000e-01 2.7424000e-01 9.9816000e-02 /
CHEB / -8.8326000e-02 -4.1935000e-02 4.8492000e-02 /
CHEB / -6.8393000e-02 -8.0203000e-02 -7.5860000e-03 /

iC4H5OJ(15)+H(+m)=tSPC(110)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2     H_rad         deltaHrxn(T=298K) = -38.79556370441571 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2002000e+00 8.2781000e-01 -3.4353000e-02 /
CHEB / -1.2529000e+00 1.1210000e+00 -2.0888000e-01 /
CHEB / -1.5516000e+00 7.4053000e-01 -3.0930000e-03 /
CHEB / -1.2307000e+00 2.2963000e-01 8.8645000e-02 /
CHEB / -8.3273000e-01 -1.1811000e-01 9.9464000e-02 /

iC4H5OJ(15)+H(+m)=C4H6O(105)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -66.98204451151231
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1221000e+01 7.3096000e-01 -9.8658000e-02 /
CHEB / -2.5148000e+00 1.2392000e+00 -1.3096000e-01 /
CHEB / -2.1928000e+00 7.3465000e-01 -6.4890000e-03 /
CHEB / -1.5053000e+00 2.1856000e-01 8.1311000e-02 /
CHEB / -9.1884000e-01 -1.2301000e-01 9.6128000e-02 /

iC4H5OJ(15)+H(+m)=C4H6Oi-13(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
92.2001629823964 kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3128000e+01 4.7093000e-01 -5.6967000e-02 /
CHEB / -1.3232000e+00 8.4873000e-01 -8.8058000e-02 /
CHEB / -1.0265000e+00 6.2163000e-01 -3.1817000e-02 /
CHEB / -7.4296000e-01 3.6727000e-01 1.6651000e-02 /
CHEB / -4.9633000e-01 1.7012000e-01 3.6128000e-02 /

iC4H5OJ(15)+H(+m)=tSPC(346)+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 16.82848295865071
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8766000e+00 -1.1315000e+00 -1.2702000e-01 /
CHEB / 6.9580000e+00 9.9938000e-01 1.4202000e-02 /
CHEB / 6.9650000e-02 2.8560000e-01 1.0028000e-01 /
CHEB / -1.1372000e-01 -3.4185000e-02 5.1694000e-02 /
CHEB / -8.1041000e-02 -7.9423000e-02 -5.6664000e-03 /

iC4H5OJ(15)+H(+m)=iC4H5OJ(14)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 1.309835166762781
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3426000e+00 -1.0470000e+00 8.8029000e-02 /
CHEB / 3.7499000e+00 7.8393000e-01 -1.7731000e-01 /
CHEB / 2.5930000e-01 3.4904000e-01 2.8978000e-03 /
CHEB / -1.6147000e-01 7.8954000e-02 9.3921000e-02 /
CHEB / -1.0044000e-01 -8.1038000e-02 3.8052000e-02 /

sC3H5+HCO(+m)=tSPC(110)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -45.96534319516243
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.0423000e+00 -5.8392000e-01 -3.2807000e-02 /
CHEB / -4.5033000e-01 1.5449000e+00 -4.5099000e-01 /
CHEB / -1.1112000e+00 1.1028000e+00 -5.3406000e-04 /
CHEB / -1.0681000e+00 3.6492000e-01 9.0079000e-02 /
CHEB / -7.7376000e-01 -4.5147000e-02 5.9158000e-02 /

sC3H5+HCO(+m)=C4H6O(105)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -74.15182400225903
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9689000e+00 -8.3975000e-01 -1.9401000e-01 /
CHEB / -1.5815000e+00 1.8831000e+00 -2.4165000e-01 /
CHEB / -1.7869000e+00 1.0412000e+00 -3.1829000e-02 /
CHEB / -1.3539000e+00 3.3326000e-01 6.6906000e-02 /
CHEB / -8.5528000e-01 -4.2446000e-02 6.0032000e-02 /

sC3H5+HCO(+m)=C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110)) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     CO_pri_rad          deltaHrxn(T=298K) = -
99.36994247314313 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.1947000e+01 6.8772000e-01 -1.1469000e-01 /
CHEB / -1.7945000e+00 1.1625000e+00 -1.4985000e-01 /
CHEB / -1.2713000e+00 7.4774000e-01 -3.0383000e-02 /
CHEB / -8.4604000e-01 3.7320000e-01 3.8461000e-02 /
CHEB / -5.3445000e-01 1.4363000e-01 4.6591000e-02 /

tSPC(346)+CH3(+m)=sC3H5+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -9.658703467903988
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1325000e+01 -1.0879000e+00 -1.3294000e-01 /
CHEB / 1.0477000e+00 1.0035000e+00 2.7447000e-02 /
CHEB / 1.1745000e-01 2.4490000e-01 1.0642000e-01 /
CHEB / -1.0466000e-01 -5.5632000e-02 4.1246000e-02 /
CHEB / -7.8408000e-02 -7.9025000e-02 -1.3690000e-02 /

iC4H5OJ(14)+H(+m)=sC3H5+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 5.859944323983941
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8495000e+00 -1.2964000e+00 -7.6051000e-02 /
CHEB / 3.7075000e+00 1.0362000e+00 -4.2802000e-02 /
CHEB / 7.4956000e-02 4.0798000e-01 7.2197000e-02 /
CHEB / -1.8277000e-01 1.3871000e-02 7.0014000e-02 /
CHEB / -1.1562000e-01 -9.1572000e-02 1.5481000e-02 /

iC4H5OJ(15)+H(+m)=sC3H5+HCO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 7.169779490746722
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4719000e+00 -1.3093000e+00 -7.4028000e-02 /
CHEB / 4.1753000e+00 1.0295000e+00 -4.5017000e-02 /
CHEB / 5.6318000e-02 4.2036000e-01 6.8277000e-02 /
CHEB / -2.0201000e-01 2.4712000e-02 7.0902000e-02 /
CHEB / -1.2765000e-01 -8.9392000e-02 1.8601000e-02 /

tSPC(110)(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -46.265194914382576
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9303000e+00 -6.6857000e-01 1.7434000e-01 /
CHEB / 1.0029000e+01 5.0199000e-01 -4.4560000e-01 /
CHEB / -4.8378000e-01 9.1313000e-01 -7.2285000e-02 /
CHEB / -8.6300000e-01 4.8897000e-01 8.3224000e-02 /
CHEB / -7.6695000e-01 3.9676000e-02 7.5145000e-02 /

C4H6O(105)(+m)=C3H6+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -18.078714107285986
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3684000e+01 -1.2784000e+00 -9.1584000e-02 /
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CHEB / 1.8908000e+01 1.2696000e+00 -1.4089000e-01 /
CHEB / -1.2049000e+00 8.4746000e-01 -5.1057000e-02 /
CHEB / -1.2404000e+00 3.7726000e-01 2.4979000e-02 /
CHEB / -8.7365000e-01 2.6592000e-02 5.2682000e-02 /

C4H6Oi-13(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = 7.139404363598107
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9135000e+01 3.2752000e-01 -2.8838000e-02 /
CHEB / 2.6536000e+01 6.0735000e-01 -4.7019000e-02 /
CHEB / -8.3507000e-01 4.8269000e-01 -2.1185000e-02 /
CHEB / -6.4183000e-01 3.2538000e-01 6.1397000e-03 /
CHEB / -4.5440000e-01 1.8153000e-01 2.3272000e-02 /

tSPC(346)+CH3(+m)=C3H6+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -101.88924157744901
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1323000e+01 -1.1650000e+00 -1.3062000e-01 /
CHEB / 8.2300000e-01 9.8667000e-01 7.0383000e-03 /
CHEB / 4.0813000e-02 3.1966000e-01 1.0006000e-01 /
CHEB / -1.0441000e-01 -1.0241000e-02 5.9979000e-02 /
CHEB / -8.3360000e-02 -7.5991000e-02 1.2695000e-03 /

iC4H5OJ(14)+H(+m)=C3H6+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -86.37059378556107
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0212000e+01 -1.4182000e+00 -5.4399000e-02 /
CHEB / 2.0321000e+00 9.5534000e-01 -5.6578000e-02 /
CHEB / 2.5448000e-01 5.1138000e-01 3.0647000e-02 /
CHEB / -1.6555000e-01 1.2982000e-01 6.5202000e-02 /
CHEB / -1.4192000e-01 -5.2022000e-02 4.1413000e-02 /

iC4H5OJ(15)+H(+m)=C3H6+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -85.06075861879829
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1077000e+01 -1.4351000e+00 -5.1125000e-02 /
CHEB / 2.2151000e+00 9.4001000e-01 -5.6703000e-02 /
CHEB / 3.0616000e-01 5.2271000e-01 2.4386000e-02 /
CHEB / -1.8412000e-01 1.4821000e-01 6.1884000e-02 /
CHEB / -1.5725000e-01 -4.2578000e-02 4.3702000e-02 /

sC3H5+HCO(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (tSPC(110))   deltaHrxn(T=298K) = -92.23053810954502
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0903000e+01 -1.3526000e+00 -6.9650000e-02 /
CHEB / 1.3130000e+00 9.9866000e-01 -5.1550000e-02 /
CHEB / 1.3473000e-01 4.5826000e-01 5.5662000e-02 /
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CHEB / -1.6091000e-01 6.8654000e-02 7.2376000e-02 /
CHEB / -1.2816000e-01 -7.3811000e-02 2.9631000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     tSPC(878)   1.93  84.58 23.61 27.25 29.83 32.1  35.87 38.32 41.05
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     iC4H5OJ(14) 14.08 76.7  22.34 26.71 30.14 32.93 37.32 40.67 46.0
!MRH CBS-QB3 w/1DHR corrections
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     CH2               93.85 46.59 8.3   8.66  8.98  9.28  9.87  10.47
      11.69
!     iC4H5OJ(15) 12.77 74.84 22.08 26.8  30.77 34.04 39.05 42.66 48.02
!MRH CBS-QB3 w/1DHR corrections
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

tSPC(878)+CH3(+m)=O2+C4H6Oi-13(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C4H6O3JJ(347))     deltaHrxn(T=298K) = -
63.8331131783132 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1615000e+00 5.4077000e-11 3.7640000e-11 /
CHEB / 3.8283000e+00 1.0607000e-10 7.3834000e-11 /
CHEB / -5.9777000e-04 9.9909000e-11 6.9541000e-11 /
CHEB / 3.1135000e-02 8.9901000e-11 6.2579000e-11 /
CHEB / 1.0661000e-02 7.6444000e-11 5.3209000e-11 /

O2+tSPC(110)(+m)=O2+C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C4H6O3JJ(347))     deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3614000e+01 1.6923000e-11 1.1778000e-11 /
CHEB / -8.3063000e-01 3.3192000e-11 2.3107000e-11 /
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CHEB / -4.0848000e-02 3.1272000e-11 2.1765000e-11 /
CHEB / -2.4077000e-02 2.8140000e-11 1.9591000e-11 /
CHEB / -2.1547000e-02 2.3931000e-11 1.6656000e-11 /

O2+tSPC(110)(+m)=tSPC(878)+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C4H6O3JJ(347))     deltaHrxn(T=298K) =
10.428513900332508 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.5664000e+00 -3.1285000e-09 -2.1777000e-09 /
CHEB / 1.8599000e+01 -6.0555000e-09 -4.2151000e-09 /
CHEB / 2.1592000e-01 -5.4865000e-09 -3.8190000e-09 /
CHEB / 5.3313000e-02 -4.6458000e-09 -3.2338000e-09 /
CHEB / -5.0059000e-03 -3.6595000e-09 -2.5473000e-09 /

iC4H5OJ(14)+HO2(+m)=O2+C4H6Oi-13(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
43.805569268693475 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7739000e+00 3.4076000e-11 2.3719000e-11 /
CHEB / 7.7340000e+00 6.6839000e-11 4.6527000e-11 /
CHEB / 3.1946000e-01 6.2957000e-11 4.3822000e-11 /
CHEB / 1.1987000e-01 5.6652000e-11 3.9435000e-11 /
CHEB / 3.7356000e-02 4.8172000e-11 3.3532000e-11 /

tSPC(878)+CH3(+m)=iC4H5OJ(14)+HO2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
20.027543909619716 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0304000e+01 -4.9467000e-09 -3.4432000e-09 /
CHEB / 1.7150000e+01 -9.5783000e-09 -6.6672000e-09 /
CHEB / 8.4716000e-01 -8.6881000e-09 -6.0476000e-09 /
CHEB / 2.7884000e-01 -7.3704000e-09 -5.1304000e-09 /
CHEB / 7.8358000e-02 -5.8203000e-09 -4.0513000e-09 /

O2+tSPC(110)(+m)=iC4H5OJ(14)+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
9.59903000928721 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2102000e+00 -2.6570000e-09 -1.8495000e-09 /
CHEB / 1.5976000e+01 -5.1365000e-09 -3.5754000e-09 /
CHEB / 5.7561000e-01 -4.6367000e-09 -3.2275000e-09 /
CHEB / 1.5512000e-01 -3.9024000e-09 -2.7164000e-09 /
CHEB / 3.0044000e-02 -3.0490000e-09 -2.1223000e-09 /

iC4H5OJ(15)+HO2(+m)=O2+C4H6Oi-13(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
42.495734101930694 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.3987000e+00 9.0526000e-09 6.2957000e-09 /
CHEB / 8.3710000e+00 1.5539000e-08 1.0814000e-08 /
CHEB / 3.1549000e-01 -5.2904000e-09 -3.6735000e-09 /
CHEB / 1.0260000e-01 -2.2023000e-08 -1.5324000e-08 /
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CHEB / 2.9356000e-02 -1.1616000e-08 -8.0903000e-09 /

tSPC(878)+CH3(+m)=iC4H5OJ(15)+HO2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
21.337379076382504 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.4729000e+00 6.5825000e-08 4.5818000e-08 /
CHEB / 1.7464000e+01 -1.1571000e-08 -8.0513000e-09 /
CHEB / 9.2919000e-01 -8.3117000e-08 -5.7857000e-08 /
CHEB / 3.0765000e-01 -3.0221000e-08 -2.1038000e-08 /
CHEB / 8.9797000e-02 1.1807000e-08 8.2192000e-09 /

O2+tSPC(110)(+m)=iC4H5OJ(15)+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
10.908865176049995 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.3808000e+00 1.3946000e-08 9.7020000e-09 /
CHEB / 1.6292000e+01 1.7804000e-08 1.2392000e-08 /
CHEB / 6.5813000e-01 -2.1919000e-08 -1.5249000e-08 /
CHEB / 1.8374000e-01 -3.7181000e-08 -2.5879000e-08 /
CHEB / 4.1317000e-02 -1.1448000e-08 -7.9747000e-09 /

iC4H5OJ(14)+HO2(+m)=iC4H5OJ(15)+HO2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (C4H6O3JJ(347))      deltaHrxn(T=298K) = -
1.3098351667627863 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6095000e+01 2.4517000e-08 1.7061000e-08 /
CHEB / 2.2545000e+01 2.2518000e-08 1.5677000e-08 /
CHEB / 1.2527000e+00 -5.0321000e-08 -3.5021000e-08 /
CHEB / 3.7459000e-01 -4.4537000e-08 -3.1005000e-08 /
CHEB / 1.0375000e-01 -6.7300000e-10 -4.7174000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     sSPC(3071)  -24.8 66.19 14.25 16.54 18.3  19.62 21.42 22.5  23.78
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
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```
sSPC(3071)+sC3H5(+m)=O2+C4H6Oi-13(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5 (C4H6O3JJ(339)) deltaHrxn(T=298K) = -
63.813731742324265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8369000e+00 1.0387000e-12 7.2146000e-13 /
CHEB / 3.0997000e+00 2.0335000e-12 1.4186000e-12 /
CHEB / 1.7723000e-01 1.9190000e-12 1.3332000e-12 /
CHEB / 6.1622000e-02 1.7242000e-12 1.2021000e-12 /
CHEB / 2.2924000e-02 1.4682000e-12 1.0205000e-12 /

O2+tSPC(110)(+m)=sSPC(3071)+sC3H5(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #5 (C4H6O3JJ(339)) deltaHrxn(T=298K) =
10.409132464343578 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7798000e+00 -8.3828000e-11 -5.8352000e-11 /
CHEB / 2.0458000e+01 -1.6356000e-10 -1.1385000e-10 /
CHEB / 2.1987000e-01 -1.5172000e-10 -1.0561000e-10 /
CHEB / 7.0044000e-02 -1.3338000e-10 -9.2846000e-11 /
CHEB / 1.9418000e-02 -1.1027000e-10 -7.6750000e-11 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     sSPC(3071)  -25.39      72.06 13.72 15.77 17.23 18.33 20.17 21.33
      22.04 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3071)+sC3H5(+m)=sSPC(2810)+CH2C[O]CH3(+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #42 (C4H6O3(1987))
      deltaHrxn(T=298K) = -77.36208661982265 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2660000e+01 -7.5234000e-05 -5.2361000e-05 /
CHEB / -1.5663000e-02 -1.1990000e-04 -8.3444000e-05 /
CHEB / -2.9056000e-02 -9.5902000e-05 -6.6741000e-05 /
CHEB / -1.7915000e-03 -7.8863000e-05 -5.4882000e-05 /
CHEB / -7.3713000e-03 -6.0357000e-05 -4.2003000e-05 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(1553)  -27.72      74.06 18.02 21.98 25.14 27.55 31.21 33.8
      35.88 null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+C2H3(+m)=C3H3O-enone+OH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #108 (C3H4O2(580)) deltaHrxn(T=298K) = -
13.419255751623643 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1192000e+00 -7.7397000e-04 -5.4055000e-04 /
CHEB / 1.1040000e+01 8.9013000e-04 6.2209000e-04 /
CHEB / 5.6509000e-01 -3.4394000e-05 -2.4491000e-05 /
CHEB / 1.8550000e-01 -6.7205000e-05 -4.7058000e-05 /
CHEB / 7.0273000e-02 -1.6625000e-05 -1.1434000e-05 /

tSPC(1553)+H(+m)=sSPC(2810)+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #108 (C3H4O2(580)) deltaHrxn(T=298K) =
12.039256411060606 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4845000e+00 -1.6418000e-03 -1.1408000e-03 /
CHEB / 5.3639000e+00 2.0774000e-03 1.4435000e-03 /
CHEB / -4.2034000e-01 -1.6239000e-04 -1.1284000e-04 /
CHEB / 1.5735000e-02 -3.5569000e-04 -2.4702000e-04 /
CHEB / 4.9355000e-02 -2.7020000e-06 -1.8565000e-06 /

O+C3H4O(+m)=C3H3O-enone+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #108 (C3H4O2(580))      deltaHrxn(T=298K) = -
19.328350813590156 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1247000e+00 -7.7255000e-04 -5.3949000e-04 /
```

```
CHEB / 9.0182000e+00 8.9549000e-04 6.2576000e-04 /
CHEB / 4.7830000e-01 -4.2264000e-05 -3.0013000e-05 /
CHEB / 1.4126000e-01 -6.7593000e-05 -4.7288000e-05 /
CHEB / 4.9286000e-02 -1.5401000e-05 -1.0574000e-05 /

tSPC(1553)+H(+m)=O+C3H4O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #108 (C3H4O2(580))      deltaHrxn(T=298K) =
17.948351473027127 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2710000e+00 -1.4707000e-03 -1.0219000e-03 /
CHEB / 6.2129000e+00 2.0410000e-03 1.4181000e-03 /
CHEB / -1.2013000e-01 -3.9216000e-04 -2.7256000e-04 /
CHEB / 4.9019000e-02 -3.5295000e-04 -2.4515000e-04 /
CHEB / 3.0373000e-02 1.1614000e-04 8.0703000e-05 /

O+C3H4O(+m)=C2H4+CO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #108 (C3H4O2(580))      deltaHrxn(T=298K) = -
120.74738584503979 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.1333000e+00 1.4506000e-02 4.4843000e-03 /
CHEB / 8.1791000e+00 -1.0627000e-02 -2.8718000e-04 /
CHEB / 6.2956000e-02 -4.7233000e-03 -3.8113000e-03 /
CHEB / -2.2669000e-02 -1.5633000e-03 -2.4468000e-03 /
CHEB / -2.8309000e-02 1.5465000e-03 1.2232000e-03 /

O+C3H4O(+m)=sSPC(2810)+C2H3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #108 (C3H4O2(580))      deltaHrxn(T=298K) = -
5.909095061966511 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0277000e+01 -1.0877000e-03 -7.5579000e-04 /
CHEB / 1.8225000e+00 1.6172000e-03 1.1236000e-03 /
CHEB / 2.7923000e-02 -5.6410000e-04 -3.9183000e-04 /
CHEB / 4.6635000e-03 -5.2621000e-05 -3.6544000e-05 /
CHEB / 2.0649000e-02 1.1770000e-04 8.1693000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!Here are the path reactions and their high-P limit kinetics:
```

```
C3H3O-enone+OH(+m)=C2H4O+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #171 (C3H4O2JJ(502))    deltaHrxn(T=298K) = -
75.92196974951793 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2987000e+01 -6.2218000e-08 -4.3308000e-08 /
CHEB / -4.4122000e-01 -1.2202000e-07 -8.4933000e-08 /
CHEB / -3.2568000e-03 -1.1486000e-07 -7.9954000e-08 /
CHEB / 1.7546000e-02 -1.0328000e-07 -7.1887000e-08 /
CHEB / 4.7205000e-03 -8.7728000e-08 -6.1066000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH4               -17.9 44.47 8.43  9.84  11.14 12.41 15.0  17.25
      20.63 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

CH3CO+OH(+m)=CO2+CH4(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #494 (C2H4O2(653))      deltaHrxn(T=298K) = -
118.97764319280337 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0781000e+01 -8.1108000e-02 -5.2922000e-02 /
CHEB / 6.8294000e-01 5.3848000e-02 3.5617000e-02 /
CHEB / 1.4056000e-02 4.2436000e-02 2.6851000e-02 /
CHEB / 2.9226000e-02 3.7222000e-04 1.7089000e-04 /
CHEB / 2.7927000e-02 -1.1660000e-02 -7.1733000e-03 /

CH3CO+OH(+m)=CH2CO+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #494 (C2H4O2(653))      deltaHrxn(T=298K) = -
76.17233098266956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1121000e+01 -8.0709000e-02 -5.2666000e-02 /
CHEB / 9.9839000e-01 5.4120000e-02 3.5792000e-02 /
CHEB / 1.0883000e-01 4.2022000e-02 2.6588000e-02 /
CHEB / 6.4732000e-02 -7.4514000e-05 -1.1144000e-04 /
CHEB / 4.1831000e-02 -1.1736000e-02 -7.2217000e-03 /
```

```
CH2CO+H2O(+m)=CO2+CH4(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #494 (C2H4O2(653))      deltaHrxn(T=298K) = -
42.805312210133806 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8123000e+00 -1.4149000e+00 -5.8999000e-02 /
CHEB / 1.6519000e+01 9.5228000e-01 -5.9478000e-02 /
CHEB / 5.8251000e-01 4.9955000e-01 3.3771000e-02 /
CHEB / -4.1626000e-02 1.2354000e-01 6.5877000e-02 /
CHEB / -5.5560000e-02 -5.1216000e-02 3.8913000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2              92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+O(+m)=CH2CHO+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1435 (C3H3O2JJJ(744))  deltaHrxn(T=298K) = -
90.25068461683392 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0724000e+01 -4.2785000e-09 -2.9782000e-09 /
CHEB / 1.3916000e+00 -8.3923000e-09 -5.8417000e-09 /
CHEB / 2.9269000e-02 -7.9047000e-09 -5.5023000e-09 /
CHEB / 1.7578000e-02 -7.1132000e-09 -4.9513000e-09 /
CHEB / 2.6410000e-03 -6.0483000e-09 -4.2101000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHO           6.29  61.8  12.81 15.33 17.49 19.29 22.06 24.11
      27.3  null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2C[O]CH3  -2.91 71.51 17.84 21.27 24.29 27.03 31.82 35.39 40.58
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     CH3CHO            -39.18      63.13 13.22 15.71 18.22 20.47 24.22
      26.97 29.78 null
!Here are the path reactions and their high-P limit kinetics:

CH2C[O]CH3+H(+m)=CH2CHO+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) = -
4.989320806555348 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1080000e+01 -4.2540000e-03 -2.9513000e-03 /
CHEB / 1.6262000e+00 4.8550000e-03 3.3653000e-03 /
CHEB / 6.5968000e-02 -6.2562000e-04 -4.3094000e-04 /
CHEB / -3.0375000e-02 -4.4230000e-04 -3.0750000e-04 /
CHEB / 6.7980000e-03 1.8273000e-05 1.2193000e-05 /

C3H6+O(+m)=CH2CHO+CH3(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) = -
23.097903886423687 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0683000e+01 -8.8954000e-04 -6.1883000e-04 /
CHEB / 1.1866000e+00 6.9080000e-04 4.8048000e-04 /
CHEB / 1.3100000e-02 1.0535000e-04 7.3284000e-05 /
CHEB / 2.2622000e-03 -1.5203000e-04 -1.0572000e-04 /
CHEB / -6.5988000e-03 -4.4567000e-05 -3.1011000e-05 /

CH2C[O]CH3+H(+m)=C3H6+O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) =
18.10858307986834 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5878000e+00 -8.8954000e-04 -6.1883000e-04 /
CHEB / 6.7582000e+00 6.9080000e-04 4.8048000e-04 /
CHEB / 8.8084000e-02 1.0535000e-04 7.3284000e-05 /
CHEB / 7.0998000e-02 -1.5203000e-04 -1.0572000e-04 /
CHEB / 3.2174000e-02 -4.4567000e-05 -3.1011000e-05 /

CH2+CH3CHO(+m)=CH2CHO+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) = -
12.058778904369987 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0689000e+01 -3.1690000e-03 -2.2003000e-03 /
CHEB / 1.2772000e+00 3.5172000e-03 2.4404000e-03 /
CHEB / 1.0124000e-01 -3.5155000e-04 -2.4260000e-04 /
CHEB / 2.7177000e-02 -4.0358000e-04 -2.8035000e-04 /
CHEB / 1.8315000e-02 1.3203000e-05 8.8065000e-06 /

CH2C[O]CH3+H(+m)=CH2+CH3CHO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) =
7.069458097814639 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6261000e+00 -3.1690000e-03 -2.2003000e-03 /
CHEB / 2.9258000e+00 3.5172000e-03 2.4404000e-03 /
CHEB / 4.3780000e-02 -3.5155000e-04 -2.4260000e-04 /
CHEB / 1.0329000e-02 -4.0358000e-04 -2.8035000e-04 /
CHEB / 8.5638000e-03 1.3203000e-05 8.8065000e-06 /

C3H6+O(+m)=CH2+CH3CHO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2026 (C3H6OJJ(768))    deltaHrxn(T=298K) = -
11.0391249820537 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0088000e+01 -8.4732000e-04 -5.8946000e-04 /
CHEB / 1.5301000e+00 6.9164000e-04 4.8107000e-04 /
CHEB / 1.4294000e-01 7.5196000e-05 5.2316000e-05 /
CHEB / 2.7813000e-02 -1.5067000e-04 -1.0478000e-04 /
CHEB / -2.6293000e-03 -3.4605000e-05 -2.4085000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(3683)  -21.17      89.45 25.88 30.32 33.98 37.23 42.49 46.51
      51.63 null
!     CH3CO       -2.28 64.25 12.39 14.28 16.26 18.05 21.06 23.24 25.14
      null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH2CO             -11.34      56.09 12.08 13.91 15.4  16.64 18.61
      20.1  22.47 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(3683)+CH3CO(+m)=C4H8O2(62)+CO2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2170 (C5H8O4(1201))     deltaHrxn(T=298K) = -
92.6505951222464 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1364000e+01 -5.2263000e-01 -1.8925000e-01 /
CHEB / 2.6811000e-01 6.1401000e-01 1.9736000e-01 /
CHEB / 8.1466000e-02 3.3945000e-03 3.6340000e-02 /
CHEB / -2.5379000e-02 -9.0252000e-02 -3.2566000e-02 /
CHEB / -7.9036000e-04 -2.8808000e-02 -2.0884000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sSPC(2810)  -38.3 60.19 9.52  11.0  12.3  13.29 15.12 16.26 15.44
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!Here are the path reactions and their high-P limit kinetics:

sSPC(2810)+tSPC(77)(+m)=CO2+C4H8O2(62)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #2382 (C5H8O4(1352))
      deltaHrxn(T=298K) = -91.84070188141828 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3606000e+00 -3.9703000e-01 -1.7202000e-01 /
CHEB / 1.1809000e+00 4.5760000e-01 1.8395000e-01 /
CHEB / 3.6733000e-01 9.1405000e-03 2.1492000e-02 /
CHEB / 7.8866000e-02 -7.1039000e-02 -2.8676000e-02 /
CHEB / 3.3973000e-02 -1.9247000e-02 -1.4168000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
```

```
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C3H5O2J(54) 21.86 78.59 23.19 28.36 32.19 35.33 39.81 42.82 47.49
      null
!Here are the path reactions and their high-P limit kinetics:

sSPC(3121)+C2H3(+m)=C3H4O+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2610 (C3H5O3J(1521))   deltaHrxn(T=298K) = -
19.887968885816925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7057000e+00 1.2908000e-09 8.9852000e-10 /
CHEB / 3.0950000e+00 2.4325000e-09 1.6932000e-09 /
CHEB / 1.0080000e-01 2.0051000e-09 1.3957000e-09 /
CHEB / 6.5992000e-03 1.4063000e-09 9.7886000e-10 /
CHEB / -2.2499000e-02 8.0402000e-10 5.5965000e-10 /

tSPC(1416)+H(+m)=sSPC(3121)+C2H3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2610 (C3H5O3J(1521))    deltaHrxn(T=298K) =
12.039256418746405 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3141000e-01 -6.6534000e-09 -4.6313000e-09 /
CHEB / 9.7565000e+00 -8.4767000e-09 -5.9004000e-09 /
CHEB / 3.2893000e-01 7.4036000e-10 5.1535000e-10 /
CHEB / 8.2631000e-02 6.2747000e-09 4.3677000e-09 /
CHEB / 8.0842000e-03 6.1867000e-09 4.3064000e-09 /

tSPC(1416)+H(+m)=C3H4O+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2610 (C3H5O3J(1521))   deltaHrxn(T=298K) = -
7.848712467070522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4647000e+00 -9.7804000e-11 -6.8080000e-11 /
CHEB / 3.7818000e+00 7.7128000e-10 5.3687000e-10 /
CHEB / -1.5177000e-01 1.6193000e-09 1.1272000e-09 /
CHEB / 1.0358000e-02 8.2371000e-10 5.7337000e-10 /
CHEB / -1.3036000e-02 -2.0673000e-10 -1.4390000e-10 /

O+C3H5O2J(54)(+m)=sSPC(3121)+C2H3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2610 (C3H5O3J(1521))    deltaHrxn(T=298K) = -
81.40150336824408 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0451000e+01 -4.3350000e-09 -3.0175000e-09 /
CHEB / 2.5101000e+00 -6.0899000e-09 -4.2390000e-09 /
CHEB / 1.2337000e-01 -6.6116000e-10 -4.6022000e-10 /
CHEB / -2.6882000e-03 3.4681000e-09 2.4141000e-09 /
CHEB / -3.4024000e-02 4.3856000e-09 3.0527000e-09 /

O+C3H5O2J(54)(+m)=C3H4O+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2610 (C3H5O3J(1521))   deltaHrxn(T=298K) = -
101.28947225406098 kcal/mol
```

```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3305000e+01 2.5147000e-09 1.7504000e-09 /
CHEB / -5.3505000e-01 4.5313000e-09 3.1542000e-09 /
CHEB / -1.6972000e-01 3.2207000e-09 2.2419000e-09 /
CHEB / -1.1576000e-01 1.5590000e-09 1.0852000e-09 /
CHEB / -7.9382000e-02 7.3848000e-11 5.1401000e-11 /

O+C3H5O2J(54)(+m)=tSPC(1416)+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2610 (C3H5O3J(1521))   deltaHrxn(T=298K) = -
93.44075978699047 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8479000e+00 -1.4494000e-09 -1.0089000e-09 /
CHEB / 7.4198000e-01 -1.6494000e-09 -1.1481000e-09 /
CHEB / -3.6927000e-01 8.8222000e-10 6.1409000e-10 /
CHEB / -1.7958000e-01 2.5588000e-09 1.7811000e-09 /
CHEB / -1.0379000e-01 2.5065000e-09 1.7447000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(343)   -9.84 83.82 25.39 30.56 34.79 38.21 43.57 47.08 51.06
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:

tSPC(343)+H(+m)=C4H6Oi-13+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2955 (C4H6O2JJ(758))   deltaHrxn(T=298K) = -
6.948946740368719 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3652000e+00 -1.7124000e-03 -1.1904000e-03 /
CHEB / 1.9838000e+00 2.1484000e-03 1.4930000e-03 /
CHEB / 3.6720000e-01 -2.8973000e-04 -2.0076000e-04 /
CHEB / 8.1345000e-02 -1.5139000e-04 -1.0543000e-04 /
CHEB / 2.9808000e-02 -1.6321000e-05 -1.1421000e-05 /

tSPC(343)+H(+m)=tSPC(110)+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2955 (C4H6O2JJ(758))   deltaHrxn(T=298K) =
46.45565253761197 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / -6.5914000e+00 -1.0973000e-04 -7.6404000e-05 /
CHEB / 1.5455000e+01 1.1848000e-04 8.2500000e-05 /
CHEB / 2.5803000e-01 7.6940000e-06 5.3507000e-06 /
CHEB / 1.5389000e-01 -1.3563000e-05 -9.4441000e-06 /
CHEB / 8.0717000e-02 -3.9094000e-06 -2.7206000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H8O2(62)+O(+m)=C4H7OJ(79)+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3118 (C4H8O3JJ(1325))  deltaHrxn(T=298K) = -
23.35731261641693 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.8307000e+00 -2.2187000e-03 -1.5425000e-03 /
CHEB / 1.7969000e+00 2.6999000e-03 1.8766000e-03 /
CHEB / 1.6665000e-01 -2.8055000e-04 -1.9434000e-04 /
CHEB / -1.3014000e-02 -1.9823000e-04 -1.3799000e-04 /
CHEB / -6.4815000e-02 -2.6934000e-05 -1.8812000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
```

```
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     H2O              -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(439)+sC3H5(+m)=C4H8O2(62)+H2CCCH3[OH](+m)  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3355 (C7H14O3(3000))
      deltaHrxn(T=298K) = -76.7121624400013 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2911000e+00 -1.0675000e-01 -6.6497000e-02 /
CHEB / 2.2933000e+00 1.2630000e-01 7.7182000e-02 /
CHEB / 7.5777000e-01 -7.1168000e-03 -2.7332000e-03 /
CHEB / 2.3117000e-01 -2.0492000e-02 -1.2820000e-02 /
CHEB / 5.5573000e-02 -8.4862000e-04 -1.0830000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O             -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3              34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     sSPC(1474)  -68.46      89.78 23.84 30.93 35.79 39.85 45.99 50.44
      55.82 null
!     sSPC(1590)  -32.7 81.02 18.05 24.1  28.23 31.69 37.16 40.84 45.44
      null
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     O                59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H7OJ(79)+sSPC(1474)(+m)=sSPC(1590)+C4H8O2(62)(+m)   1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3538 (C7H13O4J(3306))
      deltaHrxn(T=298K) = -1.2186680464765232E-7 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1235000e+01 -1.4402000e-02 -9.8241000e-03 /
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CHEB / 1.8219000e+01 1.9749000e-02 1.3435000e-02 /
CHEB / 4.2209000e-01 -4.3864000e-03 -2.9222000e-03 /
CHEB / 8.9653000e-02 -1.8614000e-03 -1.3059000e-03 /
CHEB / -8.6810000e-02 6.4423000e-04 4.3685000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     sSPC(3121)  -71.62      71.84 15.77 18.61 20.78 22.42 24.89 26.3
      27.12 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+HO2(+m)=sSPC(3121)+sC3H5(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3694 (C4H7O3J(2363))    deltaHrxn(T=298K) =
16.838397492437863 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5120000e+00 1.6206000e-09 1.1280000e-09 /
CHEB / 8.6460000e+00 3.0979000e-09 2.1564000e-09 /
CHEB / 2.3596000e-02 2.1087000e-09 1.4678000e-09 /
CHEB / -4.5487000e-02 6.1655000e-10 4.2916000e-10 /
CHEB / -5.5372000e-02 -5.5697000e-10 -3.8769000e-10 /

tSPC(110)+HO2(+m)=sSPC(3121)+sC3H5(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3694 (C4H7O3J(2363))    deltaHrxn(T=298K) = -
36.56620178554283 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0367000e+01 -1.3173000e-08 -9.1695000e-09 /
CHEB / 2.1521000e+00 -1.4886000e-08 -1.0362000e-08 /
CHEB / 1.6677000e-01 4.9956000e-09 3.4773000e-09 /
CHEB / -2.4873000e-02 1.4073000e-08 9.7960000e-09 /
CHEB / -5.9635000e-02 1.0489000e-08 7.3013000e-09 /

!PDepNetwork C5H10_iso
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C5H10_iso   -8.56 81.16 26.7  33.51 39.62 44.83 53.13 59.37 69.07
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C4H7-12           56.79 75.42 20.23 24.88 29.1  32.76 38.62 43.06
      49.99 null
!     C5H9J(7)    27.54 79.41 26.08 32.95 38.84 43.71 51.29 56.91 65.58
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     C5H9J(8)    24.43 78.2  26.21 32.6  38.22 43.01 50.67 56.38 65.23
      null
!     C5H9J(9)    40.44 84.58 25.93 32.15 37.71 42.43 49.97 55.63 64.41
      null
!     C5H9J(5)    50.54 82.55 26.51 32.76 38.26 42.91 50.31 55.88 64.54
      null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C4H7-12=C5H10_iso   1.4157154e+13      -0.15000
2.9166667e+02
!     C5H9J(7)+H=C5H10_iso    5.0000000e+13      0.00000
0.0000000e+00
!     sC3H5+C2H5=C5H10_iso    1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7+CH3=C5H10_iso     2.4874006e+15      -0.90000
2.5000000e+02
!     C5H9J(8)+H=C5H10_iso    5.0000000e+13      0.00000
0.0000000e+00
!     C5H9J(9)+H=C5H10_iso    1.0000000e+14      0.00000
0.0000000e+00
!     C5H9J(5)+H=C5H10_iso    5.3600000e+14      0.00000
9.8000000e+02

CH3+C4H7-12(+m)=C5H10_iso(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination estimate:
(Average:) C_methyl     Cd_rad/NonDe      deltaHrxn(T=298K) = -
100.58941780615494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2255000e+01 4.7509000e-01 -8.1476000e-02 /
CHEB / -9.9026000e-01 7.5647000e-01 -8.1215000e-02 /
CHEB / -6.6324000e-01 4.5854000e-01 -2.8161000e-03 /
CHEB / -3.5132000e-01 1.8829000e-01 3.8786000e-02 /
CHEB / -1.6230000e-01 2.3895000e-02 3.7764000e-02 /

C5H9J(7)+H(+m)=C5H10_iso(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
88.19049790977208 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

```
CHEB / 1.3437000e+01 3.2633000e-01 -4.6603000e-02 /
CHEB / -7.3254000e-01 5.8937000e-01 -7.5906000e-02 /
CHEB / -5.2602000e-01 4.3119000e-01 -3.6685000e-02 /
CHEB / -3.3527000e-01 2.4558000e-01 9.1233000e-04 /
CHEB / -1.8552000e-01 9.3434000e-02 2.0895000e-02 /

C5H9J(7)+H(+m)=CH3+C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = 12.398919896382871
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0244000e+00 -1.3377000e+00 -8.8459000e-02 /
CHEB / 6.7883000e+00 9.7040000e-01 -4.6839000e-02 /
CHEB / 4.9739000e-01 4.4578000e-01 5.8922000e-02 /
CHEB / -6.7944000e-02 7.1530000e-02 7.1796000e-02 /
CHEB / -1.3998000e-01 -7.4229000e-02 2.8576000e-02 /

sC3H5+C2H5(+m)=C5H10_iso(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     C_rad/H2/Cs         deltaHrxn(T=298K) = -
99.93981295484349 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2313000e+01 4.6657000e-01 -7.8857000e-02 /
CHEB / -1.0418000e+00 7.5113000e-01 -8.2371000e-02 /
CHEB / -6.6647000e-01 4.5969000e-01 -5.2288000e-03 /
CHEB / -3.6836000e-01 1.9199000e-01 3.7134000e-02 /
CHEB / -1.7377000e-01 2.6762000e-02 3.7585000e-02 /

CH3+C4H7-12(+m)=sC3H5+C2H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -0.6496048513114481
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4807000e+00 -1.2545000e+00 -1.0805000e-01 /
CHEB / 3.3420000e+00 9.9401000e-01 -2.5166000e-02 /
CHEB / 6.1875000e-01 3.8505000e-01 8.3606000e-02 /
CHEB / -4.9606000e-02 2.0377000e-02 6.9941000e-02 /
CHEB / -1.2902000e-01 -8.6163000e-02 1.3399000e-02 /

C5H9J(7)+H(+m)=sC3H5+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = 11.749315045071416
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7499000e+00 -1.3444000e+00 -8.6107000e-02 /
CHEB / 6.3773000e+00 9.7026000e-01 -4.9016000e-02 /
CHEB / 4.3682000e-01 4.4990000e-01 5.7036000e-02 /
CHEB / -9.3937000e-02 7.4637000e-02 7.1809000e-02 /
CHEB / -1.5131000e-01 -7.3584000e-02 2.9534000e-02 /

iC4H7+CH3(+m)=C5H10_iso(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_methyl       deltaHrxn(T=298K) = -
79.00173212732379 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.2535000e+01 2.7030000e-01 -3.7666000e-02 /
CHEB / -9.3129000e-01 4.9803000e-01 -6.4902000e-02 /
CHEB / -5.6614000e-01 3.8661000e-01 -3.9118000e-02 /
CHEB / -3.3898000e-01 2.4585000e-01 -1.0472000e-02 /
CHEB / -2.0288000e-01 1.1801000e-01 9.8306000e-03 /

CH3+C4H7-12(+m)=iC4H7+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -21.587685678831143
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1031000e+01 -1.3675000e+00 -8.4417000e-02 /
CHEB / 1.1868000e+00 9.4826000e-01 -5.2066000e-02 /
CHEB / 2.5948000e-01 4.6405000e-01 4.8647000e-02 /
CHEB / -1.1968000e-01 9.6972000e-02 6.9333000e-02 /
CHEB / -1.6391000e-01 -6.2441000e-02 3.3506000e-02 /

C5H9J(7)+H(+m)=iC4H7+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -9.188765782448279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0820000e+01 -1.4797000e+00 -5.4464000e-02 /
CHEB / 2.4037000e+00 8.8313000e-01 -6.8706000e-02 /
CHEB / 5.0035000e-01 5.2591000e-01 7.2522000e-03 /
CHEB / -1.5826000e-01 1.8050000e-01 5.1553000e-02 /
CHEB / -2.1114000e-01 -2.3007000e-02 4.4752000e-02 /

sC3H5+C2H5(+m)=iC4H7+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -20.93808082751969
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1041000e+01 -1.3744000e+00 -8.1995000e-02 /
CHEB / 1.1635000e+00 9.4744000e-01 -5.4090000e-02 /
CHEB / 2.6117000e-01 4.6815000e-01 4.6531000e-02 /
CHEB / -1.3758000e-01 1.0053000e-01 6.9049000e-02 /
CHEB / -1.7585000e-01 -6.1410000e-02 3.4408000e-02 /

C5H9J(8)+H(+m)=C5H10_iso(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
85.0807577853634 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3471000e+01 3.0359000e-01 -4.2857000e-02 /
CHEB / -6.9686000e-01 5.5323000e-01 -7.1680000e-02 /
CHEB / -5.0152000e-01 4.1525000e-01 -3.8428000e-02 /
CHEB / -3.2711000e-01 2.4792000e-01 -4.3590000e-03 /
CHEB / -1.9026000e-01 1.0454000e-01 1.6309000e-02 /

C5H9J(8)+H(+m)=CH3+C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = 15.508660020791545
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3457000e+00 -1.3500000e+00 -8.6597000e-02 /
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CHEB / 7.5358000e+00 9.6204000e-01 -4.9085000e-02 /
CHEB / 4.3447000e-01 4.5384000e-01 5.4706000e-02 /
CHEB / -8.1792000e-02 8.1819000e-02 7.0975000e-02 /
CHEB / -1.4760000e-01 -6.9901000e-02 3.0726000e-02 /

C5H9J(8)+H(+m)=C5H9J(7)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = 3.109740124408667
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0047000e+00 -1.4593000e+00 -5.6982000e-02 /
CHEB / 5.2811000e+00 9.0640000e-01 -6.7959000e-02 /
CHEB / 8.9574000e-01 5.1965000e-01 1.4673000e-02 /
CHEB / -3.4555000e-02 1.6099000e-01 5.7289000e-02 /
CHEB / -1.5651000e-01 -3.6889000e-02 4.4219000e-02 /

C5H9J(8)+H(+m)=sC3H5+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = 14.85905516948009
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0765000e+00 -1.3568000e+00 -8.4219000e-02 /
CHEB / 7.1196000e+00 9.6162000e-01 -5.1191000e-02 /
CHEB / 3.7404000e-01 4.5798000e-01 5.2711000e-02 /
CHEB / -1.0737000e-01 8.5111000e-02 7.0876000e-02 /
CHEB / -1.5902000e-01 -6.9108000e-02 3.1668000e-02 /

C5H9J(8)+H(+m)=iC4H7+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -6.079025658039605
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0475000e+01 -1.4950000e+00 -5.2187000e-02 /
CHEB / 2.7487000e+00 8.6560000e-01 -6.8796000e-02 /
CHEB / 5.3368000e-01 5.3017000e-01 1.7167000e-03 /
CHEB / -1.7011000e-01 1.9485000e-01 4.6848000e-02 /
CHEB / -2.2387000e-01 -1.2467000e-02 4.4676000e-02 /

C5H9J(9)+H(+m)=C5H10_iso(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination exact:
C_rad/H2/Cs     H_rad         deltaHrxn(T=298K) = -101.08918540863512
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3532000e+01 4.6657000e-01 -7.8857000e-02 /
CHEB / -9.1316000e-01 7.5113000e-01 -8.2371000e-02 /
CHEB / -6.3814000e-01 4.5969000e-01 -5.2288000e-03 /
CHEB / -3.5186000e-01 1.9199000e-01 3.7134000e-02 /
CHEB / -1.6127000e-01 2.6762000e-02 3.7585000e-02 /

C5H9J(9)+H(+m)=CH3+C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -0.49976760248016916
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.9719000e+00 -1.2545000e+00 -1.0805000e-01 /
CHEB / 3.8706000e+00 9.9401000e-01 -2.5166000e-02 /
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CHEB / 7.0908000e-01 3.8505000e-01 8.3606000e-02 /
CHEB / -2.5821000e-02 2.0377000e-02 6.9941000e-02 /
CHEB / -1.1705000e-01 -8.6163000e-02 1.3399000e-02 /

C5H9J(9)+H(+m)=C5H9J(7)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -12.898687498863048
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3633000e+00 -1.3444000e+00 -8.6107000e-02 /
CHEB / 3.1625000e+00 9.7026000e-01 -4.9016000e-02 /
CHEB / 7.8245000e-01 4.4990000e-01 5.7036000e-02 /
CHEB / 2.9789000e-02 7.4637000e-02 7.1809000e-02 /
CHEB / -1.0431000e-01 -7.3584000e-02 2.9534000e-02 /

C5H9J(9)+H(+m)=sC3H5+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -1.1493724537916243
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6609000e+00 -1.2605000e+00 -1.0603000e-01 /
CHEB / 3.5010000e+00 9.9533000e-01 -2.7664000e-02 /
CHEB / 6.4192000e-01 3.8826000e-01 8.2683000e-02 /
CHEB / -5.3818000e-02 2.2642000e-02 7.0297000e-02 /
CHEB / -1.2713000e-01 -8.6054000e-02 1.4265000e-02 /

C5H9J(9)+H(+m)=iC4H7+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -22.08745328131132
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2261000e+01 -1.3744000e+00 -8.1995000e-02 /
CHEB / 1.2922000e+00 9.4744000e-01 -5.4090000e-02 /
CHEB / 2.8950000e-01 4.6815000e-01 4.6531000e-02 /
CHEB / -1.2108000e-01 1.0053000e-01 6.9049000e-02 /
CHEB / -1.6335000e-01 -6.1410000e-02 3.4408000e-02 /

C5H9J(9)+H(+m)=C5H9J(8)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -16.00842762327172
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6762000e+00 -1.3568000e+00 -8.4219000e-02 /
CHEB / 2.7910000e+00 9.6162000e-01 -5.1191000e-02 /
CHEB / 6.8958000e-01 4.5798000e-01 5.2711000e-02 /
CHEB / 6.5125000e-03 8.5111000e-02 7.0876000e-02 /
CHEB / -1.1360000e-01 -6.9108000e-02 3.1668000e-02 /

C5H9J(5)+H(+m)=C5H10_iso(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -111.1880867105812
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3857000e+01 6.7583000e-01 -1.5155000e-01 /
CHEB / -8.7324000e-01 7.8109000e-01 -2.1673000e-02 /
CHEB / -6.8214000e-01 4.1008000e-01 4.2855000e-02 /
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CHEB / -3.3569000e-01 1.2226000e-01 5.6914000e-02 /
CHEB / -1.3270000e-01 -1.4655000e-02 3.1024000e-02 /

C5H9J(5)+H(+m)=CH3+C4H7-12(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -10.598668904426248
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0857000e+01 -1.1099000e+00 -1.5781000e-01 /
CHEB / 2.6784000e+00 9.2846000e-01 3.9470000e-02 /
CHEB / 6.5880000e-01 3.1727000e-01 9.7570000e-02 /
CHEB / 2.0686000e-02 -9.7456000e-03 5.4995000e-02 /
CHEB / -8.9223000e-02 -8.4066000e-02 -1.5624000e-03 /

C5H9J(5)+H(+m)=C5H9J(7)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -22.997588800809133
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0655000e+01 -1.1741000e+00 -1.4947000e-01 /
CHEB / 2.6174000e+00 9.1469000e-01 2.1803000e-02 /
CHEB / 6.4208000e-01 3.6681000e-01 8.5450000e-02 /
CHEB / 5.7506000e-02 2.7155000e-02 6.2348000e-02 /
CHEB / -7.0666000e-02 -7.7410000e-02 1.0204000e-02 /

C5H9J(5)+H(+m)=sC3H5+C2H5(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -11.24827375573771
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1509000e+01 -1.1137000e+00 -1.5709000e-01 /
CHEB / 2.3548000e+00 9.2882000e-01 3.8211000e-02 /
CHEB / 5.7889000e-01 3.1982000e-01 9.7122000e-02 /
CHEB / -5.6078000e-03 -8.1738000e-03 5.5472000e-02 /
CHEB / -9.9409000e-02 -8.4027000e-02 -9.9836000e-04 /

C5H9J(5)+H(+m)=iC4H7+CH3(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -32.186354583257405
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3362000e+01 -1.1978000e+00 -1.4788000e-01 /
CHEB / 9.1289000e-01 9.0213000e-01 1.5757000e-02 /
CHEB / 1.5603000e-01 3.8311000e-01 7.9943000e-02 /
CHEB / -1.0254000e-01 4.4731000e-02 6.3869000e-02 /
CHEB / -1.3055000e-01 -7.0731000e-02 1.4875000e-02 /

C5H9J(5)+H(+m)=C5H9J(8)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -26.107328925217807
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0888000e+01 -1.1838000e+00 -1.4874000e-01 /
CHEB / 2.3189000e+00 9.0995000e-01 1.9352000e-02 /
CHEB / 5.5007000e-01 3.7378000e-01 8.3235000e-02 /
CHEB / 3.0231000e-02 3.4190000e-02 6.3069000e-02 /
CHEB / -8.0162000e-02 -7.4974000e-02 1.2129000e-02 /
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C5H9J(5)+H(+m)=C5H9J(9)+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H10_iso)    deltaHrxn(T=298K) = -10.098901301946086
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8425000e+00 -1.1137000e+00 -1.5709000e-01 /
CHEB / 3.4012000e+00 9.2882000e-01 3.8211000e-02 /
CHEB / 8.5390000e-01 3.1982000e-01 9.7122000e-02 /
CHEB / 9.0736000e-02 -8.1738000e-03 5.5472000e-02 /
CHEB / -6.1486000e-02 -8.4027000e-02 -9.9836000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3OJ(9)   41.49 70.2  17.6  20.67 23.03 24.93 27.51 29.34 33.19
      null
!     HCCCHO      23.58 64.45 15.86 18.24 20.12 21.66 24.21 25.78 28.1
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H2              120.52      62.42 13.2  15.02 16.44 17.7  19.48
      20.84 24.88 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:
!     HCCCHO+H=C3H3OJ(9)      2.3501400e+11      0.30815
4.9629937e+03
!     C3H2+OH=C3H3OJ(9)       1.4157154e+13      -0.15000
2.9166667e+02

HCCCHO+H(+m)=C3H3OJ(9)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3OJ(9)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
31.08630408509729 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0091000e+01 1.7043000e-01 -5.2279000e-03 /
CHEB / 1.3095000e+00 3.2141000e-01 -7.1078000e-03 /
CHEB / -3.5384000e-01 2.6882000e-01 1.3844000e-03 /
CHEB / -2.7005000e-01 1.9781000e-01 1.1257000e-02 /
CHEB / -2.1347000e-01 1.2604000e-01 1.8489000e-02 /

C3H2+OH(+m)=C3H3OJ(9)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3OJ(9)) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     O_pri_rad       deltaHrxn(T=298K) = -
88.34068911690463 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7543000e+00 3.3195000e+00 -9.9677000e-01 /
CHEB / -3.2617000e+00 2.7508000e+00 -7.8539000e-02 /
CHEB / -1.7649000e+00 9.5565000e-01 2.5879000e-01 /
CHEB / -8.8146000e-01 2.3469000e-01 1.9231000e-01 /
CHEB / -4.6327000e-01 3.2755000e-02 8.2241000e-02 /
```

```
HCCCHO+H(+m)=C3H2+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (C3H3OJ(9))    deltaHrxn(T=298K) = 57.25438503180735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8177000e+00 -7.5489000e-01 -2.5935000e-01 /
CHEB / 1.8095000e+01 7.3977000e-01 1.7316000e-01 /
CHEB / -4.0177000e-01 1.4007000e-01 1.2277000e-01 /
CHEB / -1.7173000e-01 -3.5660000e-02 2.2880000e-02 /
CHEB / -7.4724000e-02 -4.7961000e-02 -2.0456000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
!     C3H3OJ(9)   41.49 70.2  17.6  20.67 23.03 24.93 27.51 29.34 33.19
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     pC3H3             81.58 59.57 13.76 16.14 18.14 19.8  22.39 24.34
      27.47 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(346)   27.38 68.1  17.2  20.16 22.57 24.61 27.86 30.11 33.01
      null
!Here are the path reactions and their high-P limit kinetics:
!     C3H3OJ(9)+H=C3H3OH      5.3600000e+14      0.00000
9.8000000e+02
!     pC3H3+OH=C3H3OH         1.4157154e+13      -0.15000
2.9166667e+02
!     tSPC(346)+H=C3H3OH      1.4157154e+13      -0.15000
2.9166667e+02

C3H3OJ(9)+H(+m)=C3H3OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (C3H3OH) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -85.89070166986775
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3809000e+01 4.7836000e-01 -7.9292000e-02 /
CHEB / -5.8641000e-01 7.3244000e-01 -7.0301000e-02 /
CHEB / -6.3340000e-01 4.0423000e-01 9.4608000e-03 /
CHEB / -3.2672000e-01 1.5721000e-01 3.6421000e-02 /
CHEB / -1.6754000e-01 3.4129000e-02 2.5835000e-02 /

pC3H3+OH(+m)=C3H3OH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#17 (C3H3OH) High-P Limit: R_Recombination estimate: (Average:)
Cd_pri_rad     O_pri_rad      deltaHrxn(T=298K) = -86.30084829516682
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2853000e+01 3.7657000e-01 -5.0787000e-02 /
```

```
CHEB / -1.3497000e+00 6.3805000e-01 -6.6029000e-02 /
CHEB / -6.2029000e-01 4.0062000e-01 -8.5782000e-03 /
CHEB / -3.6043000e-01 1.8617000e-01 2.2344000e-02 /
CHEB / -1.9989000e-01 5.7591000e-02 2.2457000e-02 /

C3H3OJ(9)+H(+m)=pC3H3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (C3H3OH)      deltaHrxn(T=298K) = 0.410146625299058
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2895000e+01 -1.2343000e+00 -1.0559000e-01 /
CHEB / 1.7919000e+00 9.8392000e-01 -2.2046000e-02 /
CHEB / 2.2502000e-01 3.3615000e-01 8.2933000e-02 /
CHEB / -2.2903000e-02 2.0306000e-02 5.5082000e-02 /
CHEB / -2.2450000e-02 -5.6641000e-02 8.3898000e-03 /

tSPC(346)+H(+m)=C3H3OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (C3H3OH) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     H_rad          deltaHrxn(T=298K) = -
71.78209493744552 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3015000e+01 1.8004000e-01 -1.2560000e-02 /
CHEB / -8.9130000e-01 3.3263000e-01 -2.0382000e-02 /
CHEB / -3.7386000e-01 2.6109000e-01 -9.0208000e-03 /
CHEB / -2.3455000e-01 1.7150000e-01 2.6358000e-03 /
CHEB / -1.5553000e-01 9.0799000e-02 9.4019000e-03 /

C3H3OJ(9)+H(+m)=tSPC(346)+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (C3H3OH)      deltaHrxn(T=298K) = -14.108606732422224
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2160000e+00 -1.3449000e+00 -8.5564000e-02 /
CHEB / -3.8239000e-01 9.3808000e-01 -4.4165000e-02 /
CHEB / -2.9051000e-01 4.1092000e-01 5.4351000e-02 /
CHEB / -1.8706000e-01 8.2182000e-02 5.7139000e-02 /
CHEB / -1.0358000e-01 -3.3783000e-02 2.1280000e-02 /

tSPC(346)+H(+m)=pC3H3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (C3H3OH)      deltaHrxn(T=298K) = 14.51875335772129
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4984000e+00 -1.4257000e+00 -6.1225000e-02 /
CHEB / 4.5913000e+00 9.0917000e-01 -5.6185000e-02 /
CHEB / 5.0935000e-02 4.6032000e-01 3.0944000e-02 /
CHEB / -1.0572000e-01 1.2557000e-01 5.1142000e-02 /
CHEB / -7.8006000e-02 -1.8982000e-02 2.6743000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H3OJ      41.87 70.08 16.16 18.35 20.4  22.25 25.39 27.81 31.6
      null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C3H3OJ=C4H6Oi-12    1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H5OJ(14)+H=C4H6Oi-12 5.0000000e+13      0.00000
0.0000000e+00

CH3+C3H3OJ(+m)=C4H6Oi-12(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #22 (C4H6Oi-12) High-P Limit: R_Recombination estimate:
(Average:) C_methyl     Cd_rad/NonDe      deltaHrxn(T=298K) = -
98.47655497013176 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2747000e+01 3.3506000e-01 -3.6832000e-02 /
CHEB / -1.2100000e+00 5.9692000e-01 -5.6214000e-02 /
CHEB / -6.4162000e-01 4.1972000e-01 -1.9148000e-02 /
CHEB / -3.8160000e-01 2.2545000e-01 1.0537000e-02 /
CHEB / -2.1620000e-01 8.0891000e-02 1.9732000e-02 /

iC4H5OJ(14)+H(+m)=C4H6Oi-12(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #22 (C4H6Oi-12) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     H_rad          deltaHrxn(T=298K) = -
74.35563087640004 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3940000e+01 1.3999000e-01 -9.9496000e-03 /
CHEB / -6.0410000e-01 2.6441000e-01 -1.7581000e-02 /
CHEB / -2.7254000e-01 2.2200000e-01 -1.1514000e-02 /
CHEB / -1.6267000e-01 1.6404000e-01 -3.9276000e-03 /
CHEB / -1.2343000e-01 1.0457000e-01 2.6410000e-03 /

iC4H5OJ(14)+H(+m)=CH3+C3H3OJ(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #22 (C4H6Oi-12)   deltaHrxn(T=298K) = 24.120924093731723
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1513000e+00 -1.4980000e+00 -4.2296000e-02 /
CHEB / 8.2799000e+00 8.5527000e-01 -5.2849000e-02 /
CHEB / 6.9727000e-02 5.1760000e-01 6.5235000e-03 /
CHEB / -1.6151000e-01 1.9384000e-01 3.8823000e-02 /
CHEB / -1.3554000e-01 3.6731000e-03 3.1952000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     HCCCHO      23.58 64.45 15.86 18.24 20.12 21.66 24.21 25.78 28.1
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H               134.46      51.51 10.05 10.42 10.71 10.96 11.47
      11.95 13.73 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!Here are the path reactions and their high-P limit kinetics:
!     C2H+HCO=HCCCHO          1.4157154e+13      -0.15000
2.9166667e+02

C2H+HCO(+m)=HCCCHO(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#68 (HCCCHO) High-P Limit: R_Recombination estimate: (Average:) Ct_rad
CO_pri_rad        deltaHrxn(T=298K) = -121.26734669421423 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2185000e+01 7.3594000e-01 -1.8195000e-01 /
CHEB / -1.2369000e+00 4.8742000e-01 9.2711000e-02 /
CHEB / -6.6805000e-01 3.0571000e-01 1.2395000e-02 /
CHEB / -3.0219000e-01 8.6132000e-02 1.5938000e-02 /
CHEB / -1.3985000e-01 1.5898000e-02 4.6786000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H5OJ      27.09 76.26 18.34 21.54 24.52 27.2  31.62 34.9  39.89
      null
!     CH2CHCH2O   22.15 72.99 17.7  21.45 24.85 27.83 32.58 36.01 41.06
      null
!     CHCHCH2OH   29.29 75.84 18.49 22.0  25.1  27.8  32.14 35.32 40.12
      null
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
!Here are the path reactions and their high-P limit kinetics:
!     aC3H4+OH=C3H5OJ         2.7411173e+10      0.56667
3.7888889e+03
!     C3H3OH+H=C3H5OJ         1.0000000e+13      0.00000
2.9000000e+03
!     CH2CHCH2O=C3H5OJ        2.0320555e+08      1.13906
3.4790987e+04
!     CHCHCH2OH=C3H5OJ        3.2400000e+11      0.73000
4.2400000e+04
!     C3H5OJ=C3H5O-enol2      2.8960000e+10      0.82000
3.7500000e+04
```

```
aC3H4+OH(+m)=C3H5OJ(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#93 (C3H5OJ) High-P Limit: R_Addition_MultipleBond estimate: (Average:)
Cd/H2_Ca     O_pri_rad        deltaHrxn(T=298K) = -28.946688453362754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1828000e+00 7.2180000e-01 -8.7261000e-02 /
CHEB / -6.8491000e-01 1.0414000e+00 -4.6099000e-02 /
CHEB / -1.4765000e+00 4.6142000e-01 4.3128000e-02 /
CHEB / -8.6746000e-01 8.2666000e-02 3.9516000e-02 /
CHEB / -4.5410000e-01 -5.8627000e-02 4.6334000e-03 /

C3H3OH+H(+m)=aC3H4+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C3H5OJ)      deltaHrxn(T=298K) = 2.4499873027716124
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0535000e+01 -1.1115000e+00 -9.8173000e-02 /
CHEB / 2.4721000e+00 1.0740000e+00 7.6797000e-03 /
CHEB / -8.9711000e-02 2.3361000e-01 9.9375000e-02 /
CHEB / -1.4472000e-01 -9.2806000e-02 3.6716000e-02 /
CHEB / -4.2036000e-02 -9.1639000e-02 -1.9341000e-02 /

aC3H4+OH(+m)=CH2CHCH2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C3H5OJ)      deltaHrxn(T=298K) = -33.88607643746542
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9663000e+00 -1.1424000e+00 -9.2739000e-02 /
CHEB / 2.7918000e+00 1.0710000e+00 2.3079000e-03 /
CHEB / 3.9293000e-02 2.6898000e-01 9.3099000e-02 /
CHEB / -1.2648000e-01 -7.8236000e-02 4.0568000e-02 /
CHEB / -5.2423000e-02 -9.8195000e-02 -1.4550000e-02 /

C3H5OJ(+m)=CHCHCH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C3H5OJ)      deltaHrxn(T=298K) = 2.19977537291172
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.8225000e+00 2.6442000e+00 -6.2997000e-01 /
CHEB / 1.2268000e+01 1.3573000e+00 2.4042000e-01 /
CHEB / -1.7764000e+00 3.6967000e-01 1.6445000e-01 /
CHEB / -9.7138000e-01 -1.1540000e-03 4.6981000e-02 /
CHEB / -4.8002000e-01 -8.4574000e-02 -6.7353000e-03 /

aC3H4+OH(+m)=CHCHCH2OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C3H5OJ)      deltaHrxn(T=298K) = -26.746913080451034
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5749000e+00 -5.7450000e-01 -2.1751000e-01 /
CHEB / 6.1600000e+00 6.2679000e-01 2.0348000e-01 /
CHEB / 9.4164000e-02 5.1301000e-02 6.0399000e-02 /
CHEB / -2.7720000e-02 -7.6749000e-02 -2.1738000e-02 /
CHEB / -1.6959000e-02 -3.9501000e-02 -2.5252000e-02 /
```

```
aC3H4+OH(+m)=C3H5O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #93 (C3H5OJ)      deltaHrxn(T=298K) = -57.41379585925727
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4299000e+00 -9.0341000e-01 -1.6229000e-01 /
CHEB / 4.1343000e+00 9.4432000e-01 9.6655000e-02 /
CHEB / 9.4389000e-02 1.1959000e-01 1.0086000e-01 /
CHEB / -7.5240000e-02 -1.0350000e-01 6.8221000e-03 /
CHEB / -3.6015000e-02 -6.4525000e-02 -2.9433000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H5OJ(17)  19.42 73.31 19.06 22.62 25.73 28.35 32.45 35.48 40.34
      null
!     C3H5O-enol2       -1.38 69.74 18.78 23.27 26.89 29.75 33.95 36.93
      41.61 null
!     CH3CHcOH    21.62 72.89 19.21 23.08 26.31 28.95 32.97 35.9  40.57
      null
!     C3H5OJ(12)        -1.58 70.39 18.06 21.84 25.19 28.08 32.66 36.06
      41.31 null
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     pC3H4             44.28 59.28 14.6  17.31 19.7  21.75 25.09 27.65
      32.78 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:
!     C3H3OH+H=C3H5OJ(17)     6.6800000e+13      0.00000
2.9000000e+03
!     pC3H4+OH=C3H5OJ(17)     7.6000000e+07      1.70000
1.0000000e+03
!     C3H5OJ(17)=C3H5O-enol2  2.1960000e+10      1.12000
4.1300000e+04
!     CH3CHcOH=C3H5OJ(17)     3.9400000e+11      0.69000
4.4600000e+04
!     C3H5OJ(12)=C3H5OJ(17)   2.0320555e+08      1.13906
3.4790987e+04

pC3H4+OH(+m)=C3H5OJ(17)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ct/H_Ct/Nd     O_pri_rad         deltaHrxn(T=298K)
= -34.176177301062594 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1059000e+01 1.3964000e+00 -2.1773000e-01 /
CHEB / -1.2873000e+00 6.2882000e-01 1.8614000e-01 /
CHEB / -7.5330000e-01 6.3232000e-02 6.7665000e-02 /
CHEB / -2.9959000e-01 -5.7081000e-02 -1.2594000e-02 /
CHEB / -7.5644000e-02 -3.8224000e-02 -2.1898000e-02 /
```

```
C3H3OH+H(+m)=pC3H4+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) deltaHrxn(T=298K) = 0.010182172847416737
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2420000e+01 -4.0510000e-01 -1.7359000e-01 /
CHEB / 1.3817000e+00 4.9791000e-01 1.9494000e-01 /
CHEB / 1.3398000e-02 -3.6390000e-02 1.2859000e-02 /
CHEB / 3.6320000e-03 -6.0774000e-02 -3.0830000e-02 /
CHEB / 2.9255000e-02 -9.2471000e-03 -1.0904000e-02 /

pC3H4+OH(+m)=C3H5O-enol2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) deltaHrxn(T=298K) = -54.973990729333075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.6317000e+00 -3.4124000e-01 -1.5916000e-01 /
CHEB / 3.4345000e+00 4.2477000e-01 1.8478000e-01 /
CHEB / 2.1060000e-01 -3.7942000e-02 3.3376000e-03 /
CHEB / 4.7341000e-02 -5.1381000e-02 -2.8090000e-02 /
CHEB / 2.2664000e-02 -5.7354000e-03 -7.7331000e-03 /

C3H5OJ(17)(+m)=CH3CHcOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) deltaHrxn(T=298K) = 2.199775486632589
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.7157000e+00 1.7582000e+00 -1.3050000e-01 /
CHEB / 1.3891000e+01 2.9246000e-01 1.5033000e-01 /
CHEB / -7.0257000e-01 -1.8648000e-02 1.1492000e-03 /
CHEB / -2.2111000e-01 -3.2335000e-02 -1.9174000e-02 /
CHEB / -2.4132000e-02 -6.7834000e-03 -6.1515000e-03 /

pC3H4+OH(+m)=CH3CHcOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) deltaHrxn(T=298K) = -31.976401814430005
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8361000e+00 -2.2297000e-01 -1.2065000e-01 /
CHEB / 4.7123000e+00 2.8455000e-01 1.4776000e-01 /
CHEB / 1.8732000e-01 -3.5521000e-02 -8.9061000e-03 /
CHEB / 5.9612000e-02 -3.2040000e-02 -2.0157000e-02 /
CHEB / 2.4599000e-02 -1.0442000e-03 -2.7557000e-03 /

pC3H4+OH(+m)=C3H5OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #121 (C3H5OJ(17)) deltaHrxn(T=298K) = -55.17392031081609
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1939000e+01 -5.9019000e-01 -2.1275000e-01 /
CHEB / 2.4812000e-01 6.3228000e-01 1.9008000e-01 /
CHEB / -2.6718000e-01 5.0576000e-02 6.3035000e-02 /
CHEB / -1.8281000e-01 -6.4561000e-02 -1.7571000e-02 /
CHEB / -7.6036000e-02 -3.7477000e-02 -2.2840000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
```

```
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H9Oi2     -22.94      84.64 27.11 32.27 37.18 41.54 48.7  54.18
      62.91  !MRH
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H8O-i2    -45.93      79.05 25.53 31.25 36.25 40.42 46.96 51.79
      59.42 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C4H9Oi2+O2(+m)=C4H8O-i1+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test)   deltaHrxn(T=298K) = -12.928518589081957 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2420000e+01 -8.5240000e-01 -1.5314000e-01 /
CHEB / 6.0349000e-01 9.7135000e-01 9.8310000e-02 /
CHEB / -1.2630000e-01 1.7858000e-02 9.9095000e-02 /
CHEB / -1.0955000e-01 -1.3345000e-01 -1.6364000e-02 /
CHEB / -2.0162000e-02 -2.9107000e-02 -3.2400000e-02 /

C4H9Oi2+O2(+m)=C4H8O-i2+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test)   deltaHrxn(T=298K) = -20.597812540989455 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1238000e+01 -8.5240000e-01 -1.5314000e-01 /
CHEB / -2.4573000e-01 9.7135000e-01 9.8310000e-02 /
CHEB / -3.4949000e-01 1.7858000e-02 9.9095000e-02 /
CHEB / -1.8774000e-01 -1.3345000e-01 -1.6364000e-02 /
CHEB / -5.0939000e-02 -2.9107000e-02 -3.2400000e-02 /

C4H8O-i1+HO2(+m)=C4H8O-i2+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test)   deltaHrxn(T=298K) = -7.669293951907498 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2216000e+00 -1.0928000e+00 -8.8211000e-02 /
CHEB / 3.0800000e+00 1.1252000e+00 -3.9144000e-03 /
CHEB / -1.1200000e-01 1.7458000e-01 1.0463000e-01 /
CHEB / -1.4119000e-01 -1.5465000e-01 3.1547000e-02 /
CHEB / 1.2758000e-03 -8.0492000e-02 -3.0226000e-02 /
```

```
!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H7O-N2    -13.23      80.42 21.04 25.11 28.98 32.38 37.87 42.05
      48.76
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9Oi1     -18.28      86.11 28.03 33.68 38.81 43.16 49.99 55.12
      63.33  !MRH
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C3H7O-N2+nSPC(102)(+m)=C4H9Oi1+O2(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O3J(339))  deltaHrxn(T=298K) = -
55.47451847160774 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2787000e+01 -8.2811000e-05 -6.0272000e-05 /
CHEB / -7.6211000e-01 5.2807000e-05 4.0121000e-05 /
CHEB / -2.0995000e-01 4.2101000e-05 2.8870000e-05 /
CHEB / -1.1200000e-01 4.5314000e-06 2.7528000e-06 /
CHEB / -8.0683000e-02 -8.7620000e-06 -6.0225000e-06 /

C3H7O-N2+nSPC(102)(+m)=CH3OH+aC3H5O2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O3J(339))  deltaHrxn(T=298K) = -
62.25333547718684 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 6.7514000e+00 -8.7606000e-03 -6.0735000e-03 /
CHEB / 2.0015000e+00 1.0537000e-02 7.2999000e-03 /
CHEB / 7.3372000e-01 -6.0183000e-04 -4.0984000e-04 /
CHEB / 1.8977000e-01 -1.2047000e-03 -8.3599000e-04 /
CHEB / 4.0497000e-03 -1.7975000e-04 -1.2652000e-04 /

C4H9Oi1+O2(+m)=CH3OH+aC3H5O2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -6.7788170055791035
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.4072000e+00 -1.1610000e-02 -9.5207000e-03 /
CHEB / 1.2954000e+01 1.5528000e-02 1.2820000e-02 /
CHEB / 1.3750000e-01 -2.9586000e-03 -2.5364000e-03 /
CHEB / 2.7666000e-02 -1.6392000e-03 -1.3542000e-03 /
CHEB / -1.5034000e-02 5.3479000e-04 4.6864000e-04 /

C3H7O-N2+nSPC(102)(+m)=tSPC(54)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O3J(339))  deltaHrxn(T=298K) = -
82.29191779566814 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3465000e+00 -5.2598000e-03 -3.6740000e-03 /
CHEB / 1.3020000e+00 6.0186000e-03 4.2066000e-03 /
CHEB / 4.7637000e-01 3.3393000e-05 2.0046000e-05 /
CHEB / 1.3087000e-01 -7.0835000e-04 -4.9504000e-04 /
CHEB / 1.2337000e-03 -1.8940000e-04 -1.3139000e-04 /

C4H9Oi1+O2(+m)=tSPC(54)+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -26.8173993240604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2179000e+00 -1.5524000e-01 -9.8220000e-02 /
CHEB / 7.9592000e+00 2.0083000e-01 1.2376000e-01 /
CHEB / 2.3342000e-01 -2.6339000e-02 -1.0955000e-02 /
CHEB / 5.7951000e-02 -2.5677000e-02 -1.7757000e-02 /
CHEB / 2.4349000e-03 9.7484000e-04 -1.1275000e-03 /

CH3OH+aC3H5O2(+m)=tSPC(54)+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -20.038582318481296
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2271000e+01 -3.8772000e-02 -2.6432000e-02 /
CHEB / 1.8173000e+01 4.9607000e-02 3.3687000e-02 /
CHEB / 1.0531000e+00 -6.5884000e-03 -4.2665000e-03 /
CHEB / 2.9533000e-01 -5.3352000e-03 -3.7068000e-03 /
CHEB / 5.9905000e-02 1.2546000e-04 3.6111000e-05 /

C3H7O-N2+nSPC(102)(+m)=C4H8O-i1+HO2(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O3J(339))  deltaHrxn(T=298K) = -
73.06247136479826 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0691000e+01 3.0909000e-03 1.9449000e-03 /
```

```
CHEB / -2.2952000e-02 -3.1546000e-03 -1.9272000e-03 /
CHEB / -2.0565000e-02 -4.8649000e-04 -3.6249000e-04 /
CHEB / -4.0417000e-02 2.6660000e-04 1.2799000e-04 /
CHEB / -4.9464000e-02 3.2495000e-04 2.3394000e-04 /

C4H9Oi1+O2(+m)=C4H8O-i1+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -17.58795289319052
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0396000e+01 -8.7782000e-01 -1.3778000e-01 /
CHEB / 8.2403000e-01 1.0261000e+00 8.9908000e-02 /
CHEB / -7.4228000e-03 6.4387000e-03 1.0184000e-01 /
CHEB / -9.0518000e-02 -1.4185000e-01 -2.3893000e-02 /
CHEB / -3.7029000e-02 -4.9971000e-02 -3.7530000e-02 /

CH3OH+aC3H5O2(+m)=C4H8O-i1+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -10.809135887611415
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0491000e+00 -3.1054000e-02 -2.5824000e-02 /
CHEB / 1.6214000e+01 4.0497000e-02 3.3282000e-02 /
CHEB / 4.0364000e-01 -4.6884000e-03 -3.4934000e-03 /
CHEB / 1.0897000e-01 -6.2098000e-03 -4.9317000e-03 /
CHEB / 1.9927000e-02 -3.2292000e-04 -4.5467000e-04 /

C4H8O-i1+HO2(+m)=tSPC(54)+H2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -9.229446430869885
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.5975000e+00 -2.3121000e-01 -1.3579000e-01 /
CHEB / 1.4721000e+01 2.8825000e-01 1.6401000e-01 /
CHEB / 4.3429000e-01 -2.3057000e-02 -5.7478000e-03 /
CHEB / 1.2304000e-01 -3.7908000e-02 -2.2676000e-02 /
CHEB / 3.5186000e-02 -5.4127000e-03 -5.7583000e-03 /

C3H7O-N2+nSPC(102)(+m)=C4H8O2(62)+OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H9O3J(339))  deltaHrxn(T=298K) = -
51.245181149636224 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7601000e+00 -7.5403000e-03 -6.1300000e-03 /
CHEB / 1.9760000e-01 9.8481000e-03 7.8499000e-03 /
CHEB / -1.1288000e-01 -3.6140000e-04 -1.6323000e-04 /
CHEB / -1.2408000e-01 -2.3991000e-03 -1.8684000e-03 /
CHEB / -9.1739000e-02 -2.8059000e-04 -2.4898000e-04 /

C4H8O2(62)+OH(+m)=C4H9Oi1+O2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -4.229337321971516
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4021000e+00 -1.1881000e+00 -3.6021000e-01 /
CHEB / 1.7555000e+00 1.4193000e+00 3.5446000e-01 /
CHEB / -1.7020000e-01 -3.6529000e-02 1.0015000e-01 /
```

```
CHEB / -3.0079000e-01 -1.8011000e-01 -6.1984000e-02 /
CHEB / -1.8474000e-01 -6.1987000e-02 -4.8632000e-02 /

C4H8O2(62)+OH(+m)=CH3OH+aC3H5O2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -11.008154327550617
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6185000e+00 -1.2442000e-01 -8.7548000e-02 /
CHEB / 1.2435000e+01 1.4127000e-01 9.8811000e-02 /
CHEB / 1.3098000e-01 6.7885000e-03 5.4294000e-03 /
CHEB / -6.4332000e-02 -2.0626000e-02 -1.4160000e-02 /
CHEB / -6.8138000e-02 -7.5797000e-03 -5.7137000e-03 /

C4H8O2(62)+OH(+m)=C4H8O-i1+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H9O3J(339)) deltaHrxn(T=298K) = -21.817290215162036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1833000e+01 -6.7904000e-01 -1.8983000e-01 /
CHEB / 4.0968000e-03 7.8054000e-01 1.7012000e-01 /
CHEB / -4.1367000e-01 2.6707000e-02 7.3621000e-02 /
CHEB / -3.3658000e-01 -1.0974000e-01 -2.7183000e-02 /
CHEB / -1.9300000e-01 -5.0156000e-02 -3.5522000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9Oi3     -24.24      84.93 27.12 33.12 38.42 42.88 49.87 55.11
      63.43  !MRH
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     sSPC(3121)  -68.9 67.24 17.22 19.74 21.35 22.49 24.14 25.39 27.47
!     C4H8O-i3    -51.2 79.65 23.57 29.46 34.96 39.45 46.7  51.93 57.55
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C4H8O-i2    -45.93      79.05 25.53 31.25 36.25 40.42 46.96 51.79
      59.42 null
!Here are the path reactions and their high-P limit kinetics:
```

```
C4H9Oi3+O2(+m)=C3H7-2+sSPC(3121)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (test1)   deltaHrxn(T=298K) = -19.327949535579876
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2906000e-01 -4.9281000e-01 -1.7879000e-01 /
CHEB / 6.4794000e+00 6.3872000e-01 2.0283000e-01 /
CHEB / 6.8782000e-01 -8.3266000e-02 2.0626000e-02 /
CHEB / 1.5871000e-01 -8.2619000e-02 -4.5929000e-02 /
CHEB / 4.1706000e-02 -5.5795000e-04 -1.2480000e-02 /

C4H9Oi3+O2(+m)=C4H8O-i3+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -24.56726477810644 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2272000e+00 -5.2401000e-01 -1.8352000e-01 /
CHEB / 5.7333000e+00 6.6551000e-01 2.0113000e-01 /
CHEB / 4.5561000e-01 -6.7687000e-02 3.0672000e-02 /
CHEB / 9.7110000e-02 -8.9430000e-02 -4.5562000e-02 /
CHEB / 3.0979000e-02 -7.9256000e-03 -1.7160000e-02 /

C4H8O-i3+HO2(+m)=C3H7-2+sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (test1)   deltaHrxn(T=298K) = 5.2393152425265725
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.4601000e+00 -2.1535000e-07 -1.4990000e-07 /
CHEB / 5.1080000e+00 3.2298000e-07 2.2482000e-07 /
CHEB / 3.9980000e-02 -1.1093000e-07 -7.7216000e-08 /
CHEB / 2.8433000e-02 -1.8757000e-08 -1.3056000e-08 /
CHEB / 1.5111000e-02 2.9063000e-08 2.0230000e-08 /

C4H9Oi3+O2(+m)=C4H8O-i2+HO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -19.29799768579209 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1023000e+01 -7.7142000e-01 -1.6382000e-01 /
CHEB / 4.8068000e-01 9.3814000e-01 1.3812000e-01 /
CHEB / 1.0096000e-02 -2.8020000e-02 9.2533000e-02 /
CHEB / -7.1691000e-02 -1.4568000e-01 -4.4278000e-02 /
CHEB / -1.1847000e-02 -3.7983000e-02 -4.3592000e-02 /

C4H8O-i2+HO2(+m)=C3H7-2+sSPC(3121)(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (test1)   deltaHrxn(T=298K) = -0.02995184978777843
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8732000e+00 -4.9486000e-01 -1.8604000e-01 /
CHEB / 1.3205000e+01 6.3860000e-01 2.1063000e-01 /
CHEB / 7.6545000e-01 -7.6150000e-02 2.3505000e-02 /
CHEB / 2.1816000e-01 -8.6935000e-02 -4.8629000e-02 /
CHEB / 7.7688000e-02 -4.1977000e-03 -1.5276000e-02 /

C4H8O-i2+HO2(+m)=C4H8O-i3+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -5.269267092314351 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -6.3221000e+00 -5.2584000e-01 -1.9108000e-01 /
CHEB / 1.2450000e+01 6.6346000e-01 2.0883000e-01 /
CHEB / 5.1424000e-01 -5.8044000e-02 3.4069000e-02 /
CHEB / 1.4832000e-01 -9.3381000e-02 -4.7707000e-02 /
CHEB / 6.4731000e-02 -1.2950000e-02 -2.0672000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     iC4H7OJ(30) -10.03      77.94 24.19 29.26 33.77 37.63 43.83 48.46
      55.63 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

O2+iC4H7OJ(30)(+m)=C4H6Oi-13+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(346))  deltaHrxn(T=298K) = -
14.918530328546076 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2661000e+01 -8.2455000e-01 -1.1165000e-01 /
CHEB / 5.1132000e-01 9.9223000e-01 8.5233000e-02 /
CHEB / -1.2839000e-01 -1.1845000e-02 7.2403000e-02 /
CHEB / -1.1192000e-01 -1.5926000e-01 -2.4589000e-02 /
CHEB / -2.7168000e-02 -4.6786000e-02 -3.3781000e-02 /

tSPC(110)+HO2(+m)=O2+iC4H7OJ(30)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(346))  deltaHrxn(T=298K) = -
38.48606894943461 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1491000e+01 -2.5213000e-04 -1.9695000e-04 /
CHEB / -1.6885000e-01 2.1468000e-04 1.7502000e-04 /
```

```
CHEB / -4.9061000e-02 9.6064000e-05 6.9076000e-05 /
CHEB / -1.3197000e-01 -4.5663000e-05 -4.0849000e-05 /
CHEB / -1.0185000e-01 -1.1201000e-05 -6.6291000e-06 /

tSPC(110)+HO2(+m)=C4H6Oi-13+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(346)) deltaHrxn(T=298K) = -53.40459927798069
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3516000e+01 4.1581000e-05 2.8948000e-05 /
CHEB / -1.2008000e+00 -5.4797000e-06 -3.8122000e-06 /
CHEB / -1.5940000e-01 -2.7964000e-05 -1.9469000e-05 /
CHEB / -6.1097000e-02 -1.4365000e-05 -1.0004000e-05 /
CHEB / -2.7792000e-02 -9.4838000e-07 -6.6166000e-07 /

O2+iC4H7OJ(30)(+m)=C4H6Oi-12+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(346))  deltaHrxn(T=298K) = -
9.382917146332103 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1229000e+01 -8.2478000e-01 -1.1167000e-01 /
CHEB / 1.9601000e-01 9.9228000e-01 8.5204000e-02 /
CHEB / -2.0954000e-01 -1.1542000e-02 7.2461000e-02 /
CHEB / -1.3859000e-01 -1.5924000e-01 -2.4549000e-02 /
CHEB / -3.6538000e-02 -4.6949000e-02 -3.3808000e-02 /

C4H6Oi-12+HO2(+m)=C4H6Oi-13+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(346)) deltaHrxn(T=298K) = -5.535613182213972
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1227000e+00 -9.1976000e-01 -8.9667000e-02 /
CHEB / 4.3083000e+00 1.0726000e+00 5.3063000e-02 /
CHEB / 1.5958000e-01 3.8434000e-02 7.6614000e-02 /
CHEB / -8.0112000e-03 -1.8056000e-01 -1.3729000e-02 /
CHEB / 2.7807000e-02 -7.0265000e-02 -3.4862000e-02 /

tSPC(110)+HO2(+m)=C4H6Oi-12+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(346)) deltaHrxn(T=298K) = -47.868986095766715
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2883000e+00 9.9071000e-04 6.8592000e-04 /
CHEB / 8.2959000e-01 -1.1212000e-03 -7.7627000e-04 /
CHEB / 2.1312000e-01 -8.3066000e-05 -5.5651000e-05 /
CHEB / -2.6648000e-02 2.0020000e-04 1.3486000e-04 /
CHEB / -5.1184000e-02 5.8042000e-05 4.1577000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3OH             -48.0 57.3  10.49 12.34 14.22 16.02 19.05 21.38
      25.02 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3O              4.17  57.81 9.38  11.05 12.6  14.05 16.46 18.31
      21.18 null
!Here are the path reactions and their high-P limit kinetics:
!     CH3+OH=CH3OH            6.0300000e+13      0.00000
0.0000000e+00
!     CH2OH+H=CH3OH           5.0000000e+13      0.00000
0.0000000e+00
!     CH3O+H=CH3OH            1.4157154e+13      -0.15000
2.9166667e+02

CH2OH+H(+m)=CH3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH3OH)  deltaHrxn(T=298K) = -1.2799930914562747 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3584000e+01 -2.9903000e-01 -1.6191000e-01 /
CHEB / 2.3549000e-01 3.0660000e-01 1.6141000e-01 /
CHEB / 6.3254000e-02 4.1462000e-02 2.7241000e-02 /
CHEB / 6.2351000e-02 -3.0656000e-02 -1.5595000e-02 /
CHEB / 3.9989000e-02 -2.0677000e-02 -1.1784000e-02 /

CH3O+H(+m)=CH3+OH(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH3OH)  deltaHrxn(T=298K) = -9.039395056699382 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3235000e+01 -5.1790000e-02 -4.0033000e-02 /
CHEB / -4.0322000e-01 5.6463000e-02 4.3297000e-02 /
CHEB / 1.2448000e-02 3.4927000e-03 3.1424000e-03 /
CHEB / 5.1432000e-02 -5.7775000e-03 -4.4492000e-03 /
CHEB / 3.4271000e-02 -3.1474000e-03 -2.5195000e-03 /

CH3O+H(+m)=CH2OH+H(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (CH3OH)  deltaHrxn(T=298K) = -7.759401965243107 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4955000e+00 -6.9846000e-02 -4.8240000e-02 /
CHEB / -1.6460000e+00 7.5692000e-02 5.2112000e-02 /
CHEB / -2.7804000e-01 5.3900000e-03 3.9851000e-03 /
CHEB / -4.6966000e-02 -8.0032000e-03 -5.5848000e-03 /
CHEB / -8.2376000e-03 -4.3984000e-03 -3.0916000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
```

```
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H2                0.0   -1.38 0.0   0.0   0.0   0.0   0.0   0.0
      0.0   null
!Here are the path reactions and their high-P limit kinetics:
!     HCO+H=CH2O              4.6800000e+10      0.00000     -
4.5300000e+03
!     CO+H2=CH2O              2.8900000e+09      1.16000
8.2100000e+04

HCO+H(+m)=CO+H2(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#2 (CH2O)   deltaHrxn(T=298K) = -85.81041418322731 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3382000e+00 -1.9982000e+00 -1.2230000e-03 /
CHEB / -7.5733000e-01 2.6272000e-03 -1.8098000e-03 /
CHEB / 5.3865000e-01 2.2199000e-03 -1.5284000e-03 /
CHEB / 2.8672000e-01 1.5019000e-03 -1.0316000e-03 /
CHEB / 1.0839000e-01 9.9154000e-04 -6.7955000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C3H6              4.65  63.81 15.45 19.23 22.72 25.79 30.74 34.49
      40.39 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     C3H4O-enone       -15.03      68.27 16.5  19.56 22.34 24.77 28.73
      31.72 36.36 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2+C3H4O-enone(+m)=C3H6+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C4H6OJJ(342)) deltaHrxn(T=298K) = -99.07275158845817
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0725000e+01 -5.1382000e-08 -3.5766000e-08 /
CHEB / 1.4115000e+00 -1.0076000e-07 -7.0139000e-08 /
```

```
CHEB / 3.4067000e-02 -9.4848000e-08 -6.6021000e-08 /
CHEB / 3.5567000e-02 -8.5268000e-08 -5.9353000e-08 /
CHEB / 1.1408000e-02 -7.2421000e-08 -5.0410000e-08 /

CH2+C3H4O-enone(+m)=C3H3O-enone+CH3(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C4H6OJJ(342))  deltaHrxn(T=298K) = -
31.919970858047925 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2115000e+01 -5.1382000e-08 -3.5765000e-08 /
CHEB / 1.9700000e+01 -1.0076000e-07 -7.0138000e-08 /
CHEB / 4.2079000e-01 -9.4847000e-08 -6.6021000e-08 /
CHEB / 1.7159000e-01 -8.5267000e-08 -5.9352000e-08 /
CHEB / 5.8126000e-02 -7.2420000e-08 -5.0410000e-08 /

iC4H5OJ(14)+H(+m)=CH2+C3H4O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C4H6OJJ(342))  deltaHrxn(T=298K) =
24.750973336228476 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0843000e+01 -5.1381000e-08 -3.5765000e-08 /
CHEB / 2.7614000e+01 -1.0076000e-07 -7.0138000e-08 /
CHEB / 4.3502000e-01 -9.4847000e-08 -6.6021000e-08 /
CHEB / 2.1210000e-01 -8.5266000e-08 -5.9352000e-08 /
CHEB / 9.0296000e-02 -7.2420000e-08 -5.0409000e-08 /

iC4H5OJ(14)+H(+m)=C3H3O-enone+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #9 (C4H6OJJ(342))  deltaHrxn(T=298K) = -
7.168997521819442 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2098000e+01 -5.1383000e-08 -3.5766000e-08 /
CHEB / 2.0270000e+01 -1.0076000e-07 -7.0140000e-08 /
CHEB / 5.7788000e-01 -9.4849000e-08 -6.6022000e-08 /
CHEB / 1.9218000e-01 -8.5269000e-08 -5.9353000e-08 /
CHEB / 8.2986000e-02 -7.2421000e-08 -5.0411000e-08 /

CH2+C3H4O-enone(+m)=tSPC(110)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C4H6OJJ(342)) deltaHrxn(T=298K) = -51.23761811686181
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6491000e+01 -5.1381000e-08 -3.5765000e-08 /
CHEB / 2.1484000e+01 -1.0076000e-07 -7.0138000e-08 /
CHEB / 9.5706000e-01 -9.4846000e-08 -6.6020000e-08 /
CHEB / 3.2725000e-01 -8.5266000e-08 -5.9351000e-08 /
CHEB / 1.0836000e-01 -7.2419000e-08 -5.0409000e-08 /

C3H3O-enone+CH3(+m)=tSPC(110)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #9 (C4H6OJJ(342)) deltaHrxn(T=298K) = -19.31764725881389
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2611000e+01 -5.1382000e-08 -3.5766000e-08 /
CHEB / 2.7141000e+01 -1.0076000e-07 -7.0139000e-08 /
CHEB / 7.4651000e-01 -9.4848000e-08 -6.6022000e-08 /
CHEB / 2.8215000e-01 -8.5268000e-08 -5.9353000e-08 /
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CHEB / 1.0812000e-01 -7.2421000e-08 -5.0410000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H6O             -44.5 72.73 19.42 23.41 26.92 29.97 35.32 39.17
      43.85 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C2H5              28.6  59.87 11.73 14.47 17.05 19.34 23.02 25.91
      31.53 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C3H6O-enol  -37.48      71.5  19.4  23.83 27.67 30.87 35.79 39.39
      45.1  null
!     CH3CHCHCO   2.71  74.59 22.07 26.58 30.19 33.2  37.95 41.34 45.58
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:

C3H6O-enol+CO(+m)=C3H6O+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #28 (C4H6O2JJ(466))     deltaHrxn(T=298K) = -
7.019396965630307 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0879000e+01 4.4664000e-15 1.1881000e-15 /
CHEB / 3.6442000e+01 4.5081000e-15 5.9467000e-15 /
CHEB / 3.9293000e-01 5.4452000e-15 4.5844000e-15 /
CHEB / 1.5816000e-01 8.4755000e-15 1.0831000e-15 /
CHEB / 6.3034000e-02 -9.7743000e-16 7.8880000e-15 /

CH3CHCHCO+OH(+m)=C3H6O+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #28 (C4H6O2JJ(466))     deltaHrxn(T=298K) = -
82.9413668253557 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3702000e+01 -5.1328000e-11 -3.5728000e-11 /
CHEB / 2.9545000e+01 -1.0056000e-10 -7.0001000e-11 /
CHEB / 6.3317000e-01 -9.4411000e-11 -6.5714000e-11 /
CHEB / 2.4290000e-01 -8.4530000e-11 -5.8845000e-11 /
CHEB / 9.0293000e-02 -7.1462000e-11 -4.9736000e-11 /

CH3CHCHCO+OH(+m)=C3H6O-enol+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #28 (C4H6O2JJ(466))     deltaHrxn(T=298K) = -
75.9219698597254 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3208000e+01 2.8107000e-15 -4.0560000e-17 /
CHEB / -6.2089000e-01 7.2561000e-16 3.9933000e-15 /
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CHEB / -3.1034000e-03 5.2275000e-15 -1.0378000e-16 /
CHEB / 1.9993000e-02 5.5734000e-16 3.4342000e-15 /
CHEB / 5.7820000e-03 4.0664000e-15 -1.3573000e-16 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     aC3H5             40.75 62.05 14.83 18.67 21.94 24.67 28.9  32.03
      36.9  null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     aC3H4+H=aC3H5           1.2000000e+11      0.69000
3.0000000e+03
!     pC3H5=aC3H5                   4.5900000e+10      0.97000
3.7700000e+04
!     sC3H5=aC3H5                   2.1960000e+10      1.12000
4.1300000e+04

aC3H5(+m)=pC3H5(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#106 (aC3H5)      deltaHrxn(T=298K) = 22.99758880258544 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1369000e+01 4.9820000e-01 -5.0527000e-02 /
CHEB / 1.9187000e+01 8.2535000e-01 -5.6671000e-02 /
CHEB / -1.0080000e+00 4.7585000e-01 9.8882000e-03 /
CHEB / -6.5004000e-01 1.7526000e-01 3.6636000e-02 /
CHEB / -3.6407000e-01 1.8634000e-02 2.4619000e-02 /

aC3H4+H(+m)=pC3H5(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#106 (aC3H5)      deltaHrxn(T=298K) = -31.966219657459227 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9452000e+00 -1.2357000e+00 -7.2708000e-02 /
CHEB / 3.1753000e+00 1.0787000e+00 -3.0196000e-02 /
CHEB / 2.0566000e-01 3.4201000e-01 8.2305000e-02 /
CHEB / -1.1537000e-01 -4.6063000e-02 5.6367000e-02 /
CHEB / -2.4774000e-02 -9.9737000e-02 -3.7093000e-03 /

aC3H5(+m)=sC3H5(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#106 (aC3H5)      deltaHrxn(T=298K) = 20.797813423479163 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2042000e+01 5.8406000e-01 -7.0068000e-02 /
CHEB / 1.9660000e+01 9.3362000e-01 -6.9684000e-02 /
CHEB / -1.0902000e+00 5.0571000e-01 1.5599000e-02 /
CHEB / -6.7739000e-01 1.6945000e-01 4.1682000e-02 /
CHEB / -3.7022000e-01 1.0814000e-02 2.3997000e-02 /
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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9O2J(52) -55.51      101.02      28.08 34.27 39.64 44.63 52.65
      58.11 62.84 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H8O-enol3       -35.91      84.25 23.67 29.6  34.76 39.15 46.07
      51.14 56.94 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H6O-enol2       -29.81      74.45 18.68 22.75 26.46 29.72 34.96
      38.81 44.65 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!Here are the path reactions and their high-P limit kinetics:
!     OH+C4H8O-enol3=C4H9O2J(52)    2.7100000e+12      0.00000
0.0000000e+00
!     C3H6O-enol2+CH2OH=C4H9O2J(52) 2.4100000e+10      0.00000
6.9600000e+03

OH+C4H8O-enol3(+m)=C4H9O2J(52)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #193 (C4H9O2J(52)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) O_pri_rad     Cd/H2_Cd/H/Nd      deltaHrxn(T=298K)
= -28.916791785198818 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0422000e+01 7.5285000e-01 -4.8359000e-02 /
CHEB / -5.1137000e+00 1.1181000e+00 -2.2422000e-02 /
CHEB / -3.2923000e+00 3.9242000e-01 6.0697000e-02 /
CHEB / -1.8779000e+00 -8.8934000e-02 4.9032000e-02 /
CHEB / -8.4499000e-01 -1.8620000e-01 -2.9012000e-03 /

C3H6O-enol2+CH2OH(+m)=C4H9O2J(52)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #193 (C4H9O2J(52)) High-P Limit:
R_Addition_MultipleBond estimate: (Average:) Cd/H2_Cd/H/Nd
C_rad/H2/O        deltaHrxn(T=298K) = -22.107746112712 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6376000e+00 7.5285000e-01 -4.8359000e-02 /
CHEB / -2.9006000e+00 1.1181000e+00 -2.2422000e-02 /
CHEB / -3.3134000e+00 3.9242000e-01 6.0697000e-02 /
CHEB / -1.9041000e+00 -8.8934000e-02 4.9032000e-02 /
CHEB / -8.6608000e-01 -1.8620000e-01 -2.9012000e-03 /

OH+C4H8O-enol3(+m)=C3H6O-enol2+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #193 (C4H9O2J(52)) deltaHrxn(T=298K) = -
6.809045672486816 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0441000e+01 -1.0643000e+00 -8.9703000e-02 /
CHEB / 1.0806000e+00 1.1258000e+00 1.3597000e-02 /
CHEB / -2.6930000e-01 1.7249000e-01 1.0417000e-01 /
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CHEB / -2.2159000e-01 -1.6671000e-01 2.0764000e-02 /
CHEB / -6.7561000e-02 -1.1231000e-01 -3.7260000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9O2J(53) -57.23      98.0  29.31 35.92 41.78 46.36 53.89 59.32
      65.89 null
!     C4H9O2J(54) -59.88      99.03 28.58 34.95 40.59 45.37 53.3  58.61
      65.35 null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     C2H5O-1           -7.2  70.51 14.71 17.83 20.61 23.05 26.99 29.97
      32.69 null
!     C4H8O-enol3       -35.91      84.25 23.67 29.6  34.76 39.15 46.07
      51.14 56.94 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!     cH2CH[OH]C2H3     9.75  85.19 23.45 29.19 34.08 37.79 43.84 48.16
      54.19 null
!     H2O               -57.8 45.13 8.03  8.19  8.42  8.68  9.26  9.86
      11.26 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8O-enol2       -37.68      83.04 23.93 29.26 34.16 38.51 45.56
      50.76 58.66 null
!     sC4H8O      -39.25      81.78 24.22 30.55 35.99 40.19 47.0  51.9
      58.85 null
!Here are the path reactions and their high-P limit kinetics:
!     C2H4O+C2H5O-1=C4H9O2J(53)     2.4827386e+10      0.24400
1.0487500e+04
!     C4H8O-enol3+OH=C4H9O2J(53)    2.7100000e+12      0.00000
0.0000000e+00
!     cH2CH[OH]C2H3+H2O=C4H9O2J(53) 2.2700000e+02      2.74000
5.6900000e+04
!     C4H9O2J(53)=C4H9O2J(54) 2.3600000e+10      0.82000
3.5100000e+04
!     C4H8O-enol2+OH=C4H9O2J(54)    2.7100000e+12      0.00000
0.0000000e+00
!     sC4H8O+OH=C4H9O2J(54)   2.7100000e+12      0.00000
0.0000000e+00

C4H9O2J(53)(+m)=C4H9O2J(54)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53)) High-P Limit: intra_H_migration exact:
Others-R3H_SS    C_rad_out_2H     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = -2.6496583597644303 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -6.8985000e+00 2.0825000e+00 -4.6413000e-01 /
CHEB / 4.3299000e+00 1.4840000e+00 8.8781000e-02 /
CHEB / -4.9835000e+00 6.7066000e-02 9.4332000e-02 /
CHEB / -2.6042000e+00 -4.5727000e-01 -1.0683000e-03 /
CHEB / -9.9984000e-01 -3.7126000e-01 -5.1915000e-02 /

C2H4O+C2H5O-1(+m)=C4H9O2J(53)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     C_rad/H2/Cs
      deltaHrxn(T=298K) = -20.418028256579063 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2931000e+00 9.0025000e-01 -8.4289000e-02 /
CHEB / -2.2871000e+00 1.2108000e+00 -2.9211000e-02 /
CHEB / -3.6627000e+00 3.3128000e-01 5.6194000e-02 /
CHEB / -1.9664000e+00 -1.5601000e-01 2.5728000e-02 /
CHEB / -7.7454000e-01 -2.0508000e-01 -1.6861000e-02 /

C2H4O+C2H5O-1(+m)=C4H9O2J(54)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
23.067686616343494 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.0189000e-01 1.0792000e+00 -4.6993000e-01 /
CHEB / 1.6068000e+00 2.3828000e+00 1.9325000e-01 /
CHEB / -2.8650000e+00 3.4357000e-01 1.6687000e-01 /
CHEB / -1.6754000e+00 -2.2827000e-01 1.6393000e-02 /
CHEB / -7.6873000e-01 -2.0183000e-01 -3.4616000e-02 /

C4H8O-enol3+OH(+m)=C4H9O2J(53)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H2     O_pri_rad      deltaHrxn(T=298K)
= -30.636667699856105 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7539000e+00 9.0025000e-01 -8.4289000e-02 /
CHEB / -5.7831000e+00 1.2108000e+00 -2.9211000e-02 /
CHEB / -3.6923000e+00 3.3128000e-01 5.6194000e-02 /
CHEB / -1.9731000e+00 -1.5601000e-01 2.5728000e-02 /
CHEB / -7.7783000e-01 -2.0508000e-01 -1.6861000e-02 /

C4H8O-enol3+OH(+m)=C4H9O2J(54)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
33.286326059620535 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8590000e+00 1.0792000e+00 -4.6993000e-01 /
CHEB / -1.8893000e+00 2.3828000e+00 1.9325000e-01 /
CHEB / -2.8946000e+00 3.4357000e-01 1.6687000e-01 /
CHEB / -1.6821000e+00 -2.2827000e-01 1.6393000e-02 /
CHEB / -7.7201000e-01 -2.0183000e-01 -3.4616000e-02 /

C4H8O-enol3+OH(+m)=C2H4O+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) = -
10.218639443277045 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.1417000e+01 -8.9883000e-01 -1.1644000e-01 /
CHEB / 8.4669000e-01 1.0281000e+00 7.2321000e-02 /
CHEB / -1.9411000e-01 5.2382000e-02 8.9193000e-02 /
CHEB / -1.5106000e-01 -1.5691000e-01 -1.3554000e-02 /
CHEB / -3.6786000e-02 -7.3978000e-02 -3.7474000e-02 /

C4H9O2J(53)(+m)=cH2CH[OH]C2H3+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) =
9.178806906687264 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5247000e+01 7.7263000e+00 -3.5444000e-01 /
CHEB / 1.6556000e+01 -1.7607000e-01 3.6870000e-01 /
CHEB / -3.7741000e+00 -3.5874000e-01 1.9029000e-01 /
CHEB / -1.9472000e+00 -3.3997000e-01 1.5212000e-02 /
CHEB / -7.8317000e-01 -1.5248000e-01 -5.0637000e-02 /

C4H9O2J(54)(+m)=cH2CH[OH]C2H3+H2O(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) =
11.828465266451694 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.8752000e+01 8.2210000e+00 -5.4697000e-01 /
CHEB / 1.9083000e+01 1.6577000e-01 6.3599000e-01 /
CHEB / -2.7762000e+00 -3.5528000e-01 2.5026000e-01 /
CHEB / -1.5158000e+00 -3.1883000e-01 3.1633000e-02 /
CHEB / -7.2890000e-01 -1.2712000e-01 -4.0450000e-02 /

C2H4O+C2H5O-1(+m)=cH2CH[OH]C2H3+H2O(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) = -
11.2392213498918 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0310000e+00 -1.4760000e-02 -1.2288000e-02 /
CHEB / 1.6320000e+01 1.8625000e-02 1.5492000e-02 /
CHEB / 3.4882000e-01 -1.2440000e-03 -1.0204000e-03 /
CHEB / 1.1486000e-01 -3.4429000e-03 -2.8563000e-03 /
CHEB / 3.6932000e-02 3.7821000e-05 1.5884000e-05 /

C4H8O-enol3+OH(+m)=cH2CH[OH]C2H3+H2O(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) = -
21.45786079316884 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.5701000e+00 -1.4760000e-02 -1.2288000e-02 /
CHEB / 1.2824000e+01 1.8625000e-02 1.5492000e-02 /
CHEB / 3.1922000e-01 -1.2440000e-03 -1.0204000e-03 /
CHEB / 1.0819000e-01 -3.4429000e-03 -2.8563000e-03 /
CHEB / 3.3648000e-02 3.7821000e-05 1.5884000e-05 /

C4H8O-enol2+OH(+m)=C4H9O2J(53)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
28.866830573691544 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.9029000e+00 7.3650000e-01 -3.8825000e-01 /
CHEB / -2.4209000e+00 2.2159000e+00 1.7265000e-01 /
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CHEB / -3.6485000e+00 3.0615000e-01 1.3625000e-01 /
CHEB / -2.0191000e+00 -2.8611000e-01 -1.6930000e-03 /
CHEB / -7.9115000e-01 -2.4237000e-01 -4.2937000e-02 /

C4H8O-enol2+OH(+m)=C4H9O2J(54)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/Nd     O_pri_rad
      deltaHrxn(T=298K) = -31.516488933455975 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0769000e+01 8.7522000e-01 -8.4811000e-02 /
CHEB / -4.7623000e+00 1.2020000e+00 -2.6300000e-02 /
CHEB / -2.8563000e+00 3.8349000e-01 7.3270000e-02 /
CHEB / -1.6173000e+00 -7.0417000e-02 4.4389000e-02 /
CHEB / -7.7226000e-01 -1.4916000e-01 -8.8002000e-03 /

C4H8O-enol2+OH(+m)=C2H4O+C2H5O-1(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) = -
8.448802317112484 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7207000e+00 -1.2461000e+00 -3.1694000e-01 /
CHEB / 3.9390000e+00 1.5130000e+00 3.0883000e-01 /
CHEB / 1.3665000e-02 -7.4433000e-02 9.3633000e-02 /
CHEB / -1.1081000e-01 -1.9238000e-01 -5.8898000e-02 /
CHEB / -3.3882000e-02 -4.9074000e-02 -4.2505000e-02 /

C4H8O-enol2+OH(+m)=C4H8O-enol3+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) =
1.7698371261645622 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9206000e+00 -1.2461000e+00 -3.1694000e-01 /
CHEB / 4.0871000e+00 1.5130000e+00 3.0883000e-01 /
CHEB / 5.2584000e-02 -7.4433000e-02 9.3633000e-02 /
CHEB / -9.7177000e-02 -1.9238000e-01 -5.8898000e-02 /
CHEB / -2.8515000e-02 -4.9074000e-02 -4.2505000e-02 /

C4H8O-enol2+OH(+m)=cH2CH[OH]C2H3+H2O(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #214 (C4H9O2J(53)) deltaHrxn(T=298K) = -
19.68802366700428 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.9661000e+00 -6.2518000e-02 -4.9117000e-02 /
CHEB / 1.4534000e+01 8.0509000e-02 6.3304000e-02 /
CHEB / 6.0607000e-01 -9.8500000e-03 -7.7243000e-03 /
CHEB / 1.7465000e-01 -1.1104000e-02 -8.8369000e-03 /
CHEB / 3.7240000e-02 8.1161000e-04 6.2007000e-04 /

sC4H8O+OH(+m)=C4H9O2J(53)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
27.297003747859044 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8038000e+00 6.2890000e-01 -3.8091000e-01 /
CHEB / -1.8946000e+00 2.1547000e+00 1.6785000e-01 /
CHEB / -3.6479000e+00 3.1440000e-01 1.3380000e-01 /
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CHEB / -2.0032000e+00 -2.8321000e-01 5.6235000e-04 /
CHEB / -7.7800000e-01 -2.4387000e-01 -4.2836000e-02 /

sC4H8O+OH(+m)=C4H9O2J(54)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/Nd     O_pri_rad      deltaHrxn(T=298K)
= -29.946662107623474 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1173000e+01 7.2064000e-01 -4.9573000e-02 /
CHEB / -4.6868000e+00 1.0601000e+00 -2.0467000e-02 /
CHEB / -2.7574000e+00 3.8155000e-01 5.8219000e-02 /
CHEB / -1.5848000e+00 -4.8974000e-02 4.3009000e-02 /
CHEB / -7.5759000e-01 -1.4300000e-01 -4.5688000e-03 /

sC4H8O+OH(+m)=C2H4O+C2H5O-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
6.878975491279983 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4663000e+00 -1.2855000e+00 -3.1724000e-01 /
CHEB / 4.3443000e+00 1.5480000e+00 3.0313000e-01 /
CHEB / -4.1563000e-02 -5.7228000e-02 1.0059000e-01 /
CHEB / -1.1683000e-01 -2.0013000e-01 -5.6474000e-02 /
CHEB / -2.4000000e-02 -5.6669000e-02 -4.4920000e-02 /

C4H8O-enol3+OH(+m)=sC4H8O+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
3.339663951997059 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5934000e+00 -1.2855000e+00 -3.1724000e-01 /
CHEB / 3.4966000e+00 1.5480000e+00 3.0313000e-01 /
CHEB / 7.4256000e-02 -5.7228000e-02 1.0059000e-01 /
CHEB / -6.7867000e-02 -2.0013000e-01 -5.6474000e-02 /
CHEB / 6.8267000e-04 -5.6669000e-02 -4.4920000e-02 /

sC4H8O+OH(+m)=cH2CH[OH]C2H3+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
18.118196841171788 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4342000e+00 -5.4046000e-02 -4.4312000e-02 /
CHEB / 1.5105000e+01 7.1013000e-02 5.8159000e-02 /
CHEB / 5.7307000e-01 -1.0182000e-02 -8.1970000e-03 /
CHEB / 1.7579000e-01 -1.0015000e-02 -8.2875000e-03 /
CHEB / 4.8440000e-02 1.2533000e-03 9.6205000e-04 /

C4H8O-enol2+OH(+m)=sC4H8O+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #214 (C4H9O2J(53))      deltaHrxn(T=298K) = -
1.5698268258324983 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1886000e+01 -9.8332000e-01 -1.0859000e-01 /
CHEB / 5.9945000e-01 1.0758000e+00 4.3237000e-02 /
CHEB / -1.7839000e-01 1.0573000e-01 1.0307000e-01 /
CHEB / -1.6426000e-01 -1.5328000e-01 3.9020000e-03 /
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CHEB / -4.6560000e-02 -8.1986000e-02 -3.7028000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H9O2J(55) -59.88      99.03 28.58 34.95 40.59 45.37 53.3  58.61
      65.35 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H6O-enol  -37.48      71.5  19.4  23.83 27.67 30.87 35.79 39.39
      45.1  null
!     CH2OH            -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     C4H8O-enol2      -37.68      83.04 23.93 29.26 34.16 38.51 45.56
      50.76 58.66 null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!Here are the path reactions and their high-P limit kinetics:
!     C3H6O-enol+CH2OH=C4H9O2J(55)  2.4827386e+10      0.24400
1.0487500e+04
!     C4H8O-enol2+OH=C4H9O2J(55)    2.7100000e+12      0.00000
0.0000000e+00

C3H6O-enol+CH2OH(+m)=C4H9O2J(55)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #258 (C4H9O2J(55)) High-P Limit:
R_Addition_MultipleBond estimate: (Average:) Cd/H/Nd_Cd/H/Nd
C_rad/H2/O        deltaHrxn(T=298K) = -18.807986434927876 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2994000e+00 6.6111000e-01 -4.6268000e-02 /
CHEB / 1.2045000e-01 9.9039000e-01 -1.8885000e-02 /
CHEB / -2.3060000e+00 4.0061000e-01 5.3447000e-02 /
CHEB / -1.3787000e+00 -2.7567000e-04 4.4567000e-02 /
CHEB / -7.0190000e-01 -1.2275000e-01 1.5512000e-03 /

C4H8O-enol2+OH(+m)=C4H9O2J(55)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #258 (C4H9O2J(55)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/Nd     O_pri_rad
      deltaHrxn(T=298K) = -31.516488933455975 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0778000e+01 8.0063000e-01 -8.0072000e-02 /
CHEB / -3.7312000e+00 1.1100000e+00 -1.9774000e-02 /
CHEB / -2.4181000e+00 4.0604000e-01 6.6997000e-02 /
CHEB / -1.4152000e+00 -1.7615000e-02 4.5738000e-02 /
CHEB / -7.1620000e-01 -1.2994000e-01 -2.3369000e-03 /

C4H8O-enol2+OH(+m)=C3H6O-enol+CH2OH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #258 (C4H9O2J(55)) deltaHrxn(T=298K) = -
12.708502498528096 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1267000e+01 -1.0236000e+00 -1.0805000e-01 /
CHEB / 7.8139000e-01 1.0693000e+00 3.3012000e-02 /
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CHEB / -1.5659000e-01 1.5307000e-01 1.0279000e-01 /
CHEB / -2.0355000e-01 -1.2914000e-01 1.8098000e-02 /
CHEB / -8.0159000e-02 -8.6666000e-02 -3.0234000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H5             73.78 68.69 19.31 23.54 27.01 29.83 34.14 37.35
      43.17 null
!     nC4H5             85.18 69.37 18.93 23.55 27.16 29.92 34.02 37.03
      41.81 null
!     CH3CCCH2    72.0  69.45 17.8  21.47 24.86 27.81 32.54 36.07 42.55
      null
!     C4H4-123    80.92 64.47 18.0  21.52 24.42 27.0  30.74 33.54 37.78
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H4              68.17 65.12 17.41 21.68 24.25 27.71 31.23 33.72
      37.82 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:
!     C4H4-123+H=iC4H5        5.2263889e+12      0.04600
5.0666667e+03
!     C4H4+H=iC4H5            1.8600000e+13      0.00000
2.3000000e+03
!     nC4H5=iC4H5                   2.0320555e+08      1.13906
3.4790987e+04
!     nC4H5=iC4H5                   1.9697990e+11      0.77000
4.5050000e+04
!     iC4H5=CH3CCCH2          2.0320555e+08      1.13906
3.4790987e+04
!     C4H4-123+H=CH3CCCH2     6.6800000e+13      0.00000
2.9000000e+03

iC4H5(+m)=CH3CCCH2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#364 (iC4H5) High-P Limit: intra_H_migration estimate: (Average:)
Others-R2H_S    C_rad_out_2H     XH_out         deltaHrxn(T=298K) = -
1.7796305234964507 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1657000e+00 5.7838000e-01 -3.9799000e-02 /
CHEB / 9.4879000e+00 9.8163000e-01 -4.3058000e-02 /
CHEB / -1.5641000e+00 5.7633000e-01 2.5639000e-02 /
CHEB / -1.1089000e+00 1.7414000e-01 6.1203000e-02 /
CHEB / -6.7744000e-01 -7.3418000e-02 4.6432000e-02 /

C4H4-123+H(+m)=iC4H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #364 (iC4H5) High-P Limit: R_Addition_MultipleBond estimate:
(Average:) Ca_Ca     H_rad          deltaHrxn(T=298K) = -
56.133743803504956 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0769000e+01 8.6252000e-01 -6.2208000e-01 /
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CHEB / -1.6233000e+00 3.0453000e+00 -2.5427000e-01 /
CHEB / -1.8549000e+00 1.1064000e+00 1.3634000e-01 /
CHEB / -1.0733000e+00 2.0983000e-01 1.4143000e-01 /
CHEB / -5.9364000e-01 -9.2839000e-02 5.9698000e-02 /

C4H4-123+H(+m)=CH3CCCH2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #364 (iC4H5) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Ca     H_rad      deltaHrxn(T=298K) = -57.91337432700141 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1542000e+01 1.6673000e+00 -4.1587000e-01 /
CHEB / -2.3504000e+00 2.1999000e+00 -3.6147000e-01 /
CHEB / -1.7301000e+00 9.6595000e-01 1.1859000e-02 /
CHEB / -9.3946000e-01 2.8321000e-01 1.1098000e-01 /
CHEB / -5.0843000e-01 -5.6422000e-03 8.9072000e-02 /

C4H4+H(+m)=iC4H5(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#364 (iC4H5) High-P Limit: R_Addition_MultipleBond exact:  Ct/H_Ct/De
H_rad       deltaHrxn(T=298K) = -43.3851424434969 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2012000e+01 8.8102000e-01 -1.6568000e-01 /
CHEB / -1.9785000e+00 1.3251000e+00 -1.5274000e-01 /
CHEB / -1.4949000e+00 7.2563000e-01 -7.4264000e-03 /
CHEB / -9.2598000e-01 2.6623000e-01 4.9446000e-02 /
CHEB / -5.4059000e-01 6.1934000e-03 5.1411000e-02 /

C4H4+H(+m)=CH3CCCH2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#364 (iC4H5)      deltaHrxn(T=298K) = -45.164772966993354 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0763000e+01 -3.8713000e-01 -2.5404000e-01 /
CHEB / -5.6555000e-01 2.3540000e+00 -1.9542000e-01 /
CHEB / -1.2623000e+00 1.0592000e+00 8.6310000e-02 /
CHEB / -9.3011000e-01 2.4565000e-01 1.1883000e-01 /
CHEB / -5.5143000e-01 -6.3672000e-02 5.2482000e-02 /

C4H4-123+H(+m)=C4H4+H(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #364 (iC4H5)      deltaHrxn(T=298K) = -12.748601360008045
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.4613000e+00 -1.9389000e+00 -2.5388000e-01 /
CHEB / 4.0035000e-01 1.8027000e+00 4.0480000e-02 /
CHEB / -3.9563000e-01 3.8931000e-01 2.1048000e-01 /
CHEB / -2.9383000e-01 -7.0108000e-02 8.6473000e-02 /
CHEB / -1.7155000e-01 -1.2111000e-01 -2.4014000e-02 /

iC4H5(+m)=nC4H5(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#364 (iC4H5)      deltaHrxn(T=298K) = 11.398915866472805 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.1020000e+00 7.8039000e-01 -1.3399000e-01 /
CHEB / 1.4417000e+01 1.2202000e+00 -1.3729000e-01 /
CHEB / -1.0608000e+00 6.8322000e-01 -5.5297000e-03 /
CHEB / -8.2346000e-01 2.5602000e-01 4.7178000e-02 /
CHEB / -5.2231000e-01 1.1208000e-02 4.6781000e-02 /
```

```
CH3CCCH2(+m)=nC4H5(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#364 (iC4H5)      deltaHrxn(T=298K) = 13.178546389969256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0270000e+01 -5.1053000e-01 -2.1578000e-01 /
CHEB / 1.6804000e+01 2.2408000e+00 -1.8223000e-01 /
CHEB / -7.2874000e-01 1.0424000e+00 7.8028000e-02 /
CHEB / -8.2493000e-01 2.4853000e-01 1.1779000e-01 /
CHEB / -5.3875000e-01 -6.2570000e-02 5.3881000e-02 /

C4H4-123+H(+m)=nC4H5(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #364 (iC4H5)      deltaHrxn(T=298K) = -44.73482793703215
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0015000e+01 -1.9475000e+00 -2.5940000e-01 /
CHEB / 3.6475000e+00 1.8044000e+00 4.5041000e-02 /
CHEB / 4.5486000e-01 3.9560000e-01 2.1027000e-01 /
CHEB / 9.9641000e-03 -6.6912000e-02 8.7478000e-02 /
CHEB / -5.2151000e-02 -1.2102000e-01 -2.2637000e-02 /

!PDepNetwork C5H8(95)
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C5H8(95)    17.98 75.23 25.25 31.72 37.1  41.39 48.01 52.92 60.66
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H5             86.31 99.28 18.52 22.6  26.13 29.08 33.64 37.01
      42.26
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!Here are the path reactions and their high-P limit kinetics:
!     CH3+iC4H5=C5H8(95)      1.4157154e+13      -0.15000
2.9166667e+02
!     sC3H5+C2H3=C5H8(95)     7.2300000e+13      0.00000
0.0000000e+00

CH3+iC4H5(+m)=C5H8(95)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H8(95)) High-P Limit: R_Recombination estimate:
(Average:) C_methyl     Cd_rad/OneDe      deltaHrxn(T=298K) = -
103.56912773111485 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0439000e+01 7.8725000e-01 -6.7803000e-02 /
CHEB / -3.8404000e+00 9.4764000e-01 1.3539000e-02 /
CHEB / -2.5626000e+00 3.0527000e-01 3.9807000e-02 /
CHEB / -1.5150000e+00 3.2177000e-02 1.5858000e-02 /
CHEB / -8.9611000e-01 -1.2304000e-02 -5.2620000e-04 /
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sC3H5+C2H3(+m)=C5H8(95)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H8(95)) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     Cd_pri_rad          deltaHrxn(T=298K) = -
116.1682024003171 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0734000e+00 3.5946000e+00 -2.1882000e-01 /
CHEB / -4.4534000e+00 2.2880000e-01 8.1166000e-02 /
CHEB / -2.7193000e+00 1.1913000e-01 4.4375000e-02 /
CHEB / -1.5032000e+00 2.0720000e-02 1.6565000e-03 /
CHEB / -8.7961000e-01 -6.8673000e-03 -3.1371000e-03 /

sC3H5+C2H3(+m)=CH3+iC4H5(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C5H8(95))     deltaHrxn(T=298K) = -12.599074669202238
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3943000e+01 -4.8833000e-02 -3.4625000e-02 /
CHEB / -3.8018000e-02 6.7724000e-02 4.8008000e-02 /
CHEB / -7.8049000e-03 -1.5357000e-02 -1.0990000e-02 /
CHEB / 1.1196000e-02 -7.5598000e-03 -5.0847000e-03 /
CHEB / 7.1106000e-03 3.4465000e-03 2.2676000e-03 /

!PDepNetwork C4H4
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H4              71.86 66.24 17.18 20.88 23.88 26.32 30.06 32.83
      37.25
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H               137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     iC4H3             121.56      70.27 18.68 21.24 23.29 24.97 27.64
      29.68 32.95
!     nC4H3             132.99      67.35 17.24 20.41 22.8  24.66 27.47
      29.56 32.87
!Here are the path reactions and their high-P limit kinetics:
!     C2H+C2H3=C4H4           1.0000000e+14      0.00000
0.0000000e+00
!     iC4H3+H=C4H4            1.4157154e+13      -0.15000
2.9166667e+02
!     nC4H3+H=C4H4            1.000e+14    0.00        0.00

C2H+C2H3(+m)=C4H4(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H4) High-P Limit: R_Recombination exact:  Ct_rad     Cd_pri_rad
      deltaHrxn(T=298K) = -137.46558408335005 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2765000e+01 1.1573000e+00 -2.3009000e-01 /
CHEB / -1.3983000e+00 7.4463000e-01 1.2652000e-01 /
CHEB / -7.2939000e-01 1.7217000e-01 1.0189000e-01 /
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CHEB / -2.9024000e-01 -2.1342000e-02 2.4191000e-02 /
CHEB / -9.3672000e-02 -4.7485000e-02 -1.3527000e-02 /

iC4H3+H(+m)=C4H4(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H4) High-P Limit: R_Recombination estimate: (Average:)
Cd_rad/OneDe     H_rad        deltaHrxn(T=298K) = -101.78874562826662
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2302000e+01 3.2345000e-01 -6.7435000e-02 /
CHEB / -5.7095000e-01 5.6108000e-01 -9.9249000e-02 /
CHEB / -4.7911000e-01 3.8442000e-01 -3.9563000e-02 /
CHEB / -2.7451000e-01 2.0061000e-01 7.8910000e-03 /
CHEB / -1.5021000e-01 6.5887000e-02 2.7699000e-02 /

C2H+C2H3(+m)=iC4H3+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H4)   deltaHrxn(T=298K) = -35.676838455083406 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3267000e+01 -8.0336000e-01 -2.1937000e-01 /
CHEB / 4.4551000e-01 7.6796000e-01 1.4327000e-01 /
CHEB / -3.5657000e-02 1.4712000e-01 1.0053000e-01 /
CHEB / -7.5175000e-02 -4.7361000e-02 1.2257000e-02 /
CHEB / -5.3667000e-02 -5.6324000e-02 -2.2297000e-02 /

nC4H3+H(+m)=C4H4(+m)    1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H4) High-P Limit: R_Recombination Primary Kinetic Library: MRH
      deltaHrxn(T=298K) = -113.21784552214469 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3630000e+01 4.6946000e-01 -8.7279000e-02 /
CHEB / -9.7103000e-01 7.5733000e-01 -9.9904000e-02 /
CHEB / -6.0874000e-01 4.3494000e-01 -2.5087000e-03 /
CHEB / -3.1940000e-01 1.6194000e-01 4.5055000e-02 /
CHEB / -1.4430000e-01 1.2018000e-02 4.0734000e-02 /

C2H+C2H3(+m)=nC4H3+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H4)   deltaHrxn(T=298K) = -24.247738561205345 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2724000e+01 -7.9005000e-01 -2.1653000e-01 /
CHEB / 7.3790000e-01 7.7224000e-01 1.4762000e-01 /
CHEB / 8.7920000e-02 1.3547000e-01 9.8703000e-02 /
CHEB / -2.9430000e-02 -5.5917000e-02 7.6790000e-03 /
CHEB / -3.4800000e-02 -5.7451000e-02 -2.4676000e-02 /

nC4H3+H(+m)=iC4H3+H(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (C4H4)   deltaHrxn(T=298K) = -11.429099893878053 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2136000e+01 -1.3736000e+00 -7.9286000e-02 /
CHEB / 1.6480000e+00 9.6540000e-01 -6.2061000e-02 /
CHEB / 2.7268000e-01 4.5833000e-01 5.0228000e-02 /
CHEB / -9.2114000e-02 8.1815000e-02 7.3487000e-02 /
CHEB / -1.0465000e-01 -6.7965000e-02 3.3472000e-02 /

!PDepNetwork
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!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H5-113          74.45 69.13 18.96 22.67 25.88 28.64 33.04 36.35
      43.49 null
!     C4H5-114    88.55 72.99 18.78 22.51 25.72 28.43 32.79 36.1  42.32
      null
!     C4H4              68.17 65.12 17.41 21.68 24.25 27.71 31.23 33.72
      37.82 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H2              120.52      62.42 13.2  15.02 16.44 17.7  19.48
      20.84 24.88 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:
!     C4H4+H=C4H5-113         3.7100000e+13      0.00000
1.0000000e+03
!     C3H2+CH3=C4H5-113       7.2300000e+13      0.00000
0.0000000e+00
!     C4H5-114=C4H5-113       5.6400000e+08      1.28000
2.7900000e+04

C4H4+H(+m)=C4H5-113(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#828 (C4H5-113) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H/De     H_rad       deltaHrxn(T=298K) = -42.71515192615486
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2411000e+01 6.5690000e-01 -9.0088000e-02 /
CHEB / -1.0216000e+00 9.5732000e-01 -5.1918000e-02 /
CHEB / -8.2002000e-01 4.2066000e-01 5.8859000e-02 /
CHEB / -3.3717000e-01 6.5542000e-02 6.6800000e-02 /
CHEB / -8.9596000e-02 -5.9564000e-02 2.4699000e-02 /

C3H2+CH3(+m)=C4H5-113(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #828 (C4H5-113) High-P Limit: R_Recombination exact:
Cd_pri_rad     C_methyl       deltaHrxn(T=298K) = -80.87133663797862
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2281000e+01 1.6494000e+00 -1.7143000e-01 /
CHEB / -2.0930000e+00 3.9604000e-01 1.7791000e-01 /
CHEB / -7.6627000e-01 5.1108000e-03 2.2949000e-02 /
CHEB / -2.3609000e-01 -4.1486000e-02 -2.0162000e-02 /
CHEB / -3.3632000e-02 -1.7877000e-02 -1.3357000e-02 /

C4H4+H(+m)=C3H2+CH3(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#828 (C4H5-113)   deltaHrxn(T=298K) = 38.15618471182375 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9623000e+00 -3.4215000e-01 -1.6724000e-01 /
CHEB / 1.1184000e+01 3.9667000e-01 1.7930000e-01 /
CHEB / -3.8016000e-01 -3.6532000e-03 1.8370000e-02 /
CHEB / -1.2860000e-01 -4.5061000e-02 -2.2916000e-02 /
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CHEB / -2.9961000e-02 -1.5876000e-02 -1.2640000e-02 /

C4H5-113(+m)=C4H5-114(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #828 (C4H5-113)   deltaHrxn(T=298K) = 14.098579888093553
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.4868000e+00 5.2703000e-01 -5.4739000e-02 /
CHEB / 1.3288000e+01 8.6624000e-01 -5.9364000e-02 /
CHEB / -7.2614000e-01 4.8036000e-01 1.7484000e-02 /
CHEB / -4.2182000e-01 1.5141000e-01 4.7304000e-02 /
CHEB / -1.7866000e-01 -1.3097000e-02 3.0380000e-02 /

C4H4+H(+m)=C4H5-114(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#828 (C4H5-113)   deltaHrxn(T=298K) = -28.616572038061307 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1871000e+01 -1.1888000e+00 -9.8308000e-02 /
CHEB / 1.7618000e+00 1.0687000e+00 -1.9239000e-02 /
CHEB / 1.0532000e-01 3.0671000e-01 1.0025000e-01 /
CHEB / -9.4338000e-02 -6.4724000e-02 5.9253000e-02 /
CHEB / -4.3456000e-02 -1.0412000e-01 -9.0184000e-03 /

C3H2+CH3(+m)=C4H5-114(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #828 (C4H5-113)   deltaHrxn(T=298K) = -66.77275674988506
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4019000e+01 -3.4357000e-01 -1.6793000e-01 /
CHEB / -3.9483000e-01 3.9668000e-01 1.7913000e-01 /
CHEB / -1.7414000e-01 -2.1446000e-03 1.9163000e-02 /
CHEB / -7.8149000e-02 -4.4557000e-02 -2.2505000e-02 /
CHEB / -2.7988000e-02 -1.6287000e-02 -1.2810000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H4-123    80.92 64.47 18.0  21.52 24.42 27.0  30.74 33.54 37.78
      null
!     iC4H3             117.82      68.51 17.55 20.47 22.78 24.85 27.76
      29.94 34.18 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     iC4H3+H=C4H4-123        5.3600000e+14      0.00000
9.8000000e+02

iC4H3+H(+m)=C4H4-123(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #912 (C4H4-123) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -85.89070174742362
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4547000e+01 2.5952000e-02 -1.3430000e-02 /
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CHEB / 1.7434000e-01 4.9999000e-02 -2.5770000e-02 /
CHEB / -7.3226000e-03 4.4732000e-02 -2.2782000e-02 /
CHEB / 3.3990000e-02 3.7207000e-02 -1.8587000e-02 /
CHEB / 1.4506000e-02 2.8738000e-02 -1.3992000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nC4H3             127.27      66.51 17.22 20.93 22.89 25.79 28.41
      30.23 33.29 null
!     iC4H3             117.82      68.51 17.55 20.47 22.78 24.85 27.76
      29.94 34.18 null
!     C2H               134.46      51.51 10.05 10.42 10.71 10.96 11.47
      11.95 13.73 null
!     C2H2              53.86 48.02 10.56 11.98 12.98 13.74 14.94 15.92
      17.7  null
!     C4H2              105.06      59.78 17.64 20.1  21.78 23.02 24.94
      26.38 28.84 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     C2H+C2H2=nC4H3          5.0000000e+12      0.00000
0.0000000e+00
!     C4H2+H=nC4H3            2.2500000e+13      0.00000
5.4000000e+03
!     nC4H3=iC4H3                   1.9697990e+11      0.77000
4.5050000e+04

C2H+C2H2(+m)=nC4H3(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1145 (nC4H3) High-P Limit: R_Addition_MultipleBond exact:  Ct_rad
Ct/H_Ct/H         deltaHrxn(T=298K) = -61.04334362136467 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8437000e+00 4.8349000e+00 -1.0442000e+00 /
CHEB / -4.0077000e+00 1.5083000e+00 5.6260000e-01 /
CHEB / -2.0677000e+00 2.7456000e-01 2.5618000e-01 /
CHEB / -1.0057000e+00 -6.3931000e-02 6.8866000e-02 /
CHEB / -4.9753000e-01 -1.1080000e-01 1.0184000e-02 /

C4H2+H(+m)=C2H+C2H2(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1145 (nC4H3)     deltaHrxn(T=298K) = 34.25686654183801 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9571000e+00 -3.1465000e-01 -1.8192000e-01 /
CHEB / 9.8896000e+00 3.8372000e-01 2.0512000e-01 /
CHEB / -4.4266000e-01 -1.4263000e-02 1.4818000e-02 /
CHEB / -1.1985000e-01 -5.4009000e-02 -3.0825000e-02 /
CHEB / -2.5929000e-02 -1.4101000e-02 -1.4219000e-02 /

nC4H3(+m)=iC4H3(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1145 (nC4H3) High-P Limit: intra_H_migration estimate: (Average:) R2H_D
Cd_rad_out_singleH     Cd_H_out_singleDe        deltaHrxn(T=298K) = -
9.44909553433294 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / -6.3002000e+00 1.5184000e+00 -4.7096000e-01 /
CHEB / 1.2758000e+01 1.4557000e+00 -1.2859000e-01 /
CHEB / -1.4702000e+00 5.6461000e-01 6.2707000e-02 /
CHEB / -8.6674000e-01 9.4045000e-02 6.8932000e-02 /
CHEB / -4.7043000e-01 -6.6092000e-02 2.7112000e-02 /

C2H+C2H2(+m)=iC4H3(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1145 (nC4H3)     deltaHrxn(T=298K) = -70.49243915569761 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2506000e+01 -3.6241000e-01 -1.8232000e-01 /
CHEB / 1.9092000e-01 4.2996000e-01 1.9993000e-01 /
CHEB / -3.3425000e-02 -1.0270000e-02 1.7815000e-02 /
CHEB / -1.1354000e-02 -5.5529000e-02 -2.8496000e-02 /
CHEB / 1.3967000e-03 -1.3425000e-02 -1.2889000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7O-14    7.38  85.17 24.32 29.59 34.01 37.72 43.55 47.83 52.47
      null
!     C4H7O-13          -2.41 80.44 22.13 27.78 32.68 36.83 43.32 48.0
      53.09 null
!     C4H7O_1_2   -8.74 77.49 22.98 28.87 33.91 38.04 44.26 48.73 55.61
      null
!     C4H7OJ(9)   6.76  84.71 23.75 29.33 34.08 37.96 43.85 48.13 54.8
      null
!     C4H7OJ(12)        -6.34 80.19 23.18 28.7  33.51 37.57 43.88 48.54
      55.67 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     CH2CHCHCHOH -16.05      75.67 23.07 28.9  33.47 36.92 41.89 45.42
      51.05 null
!     C4H6-13           26.08 66.6  19.12 24.3  28.52 31.84 36.84 40.52
      46.34 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH3CHCHCHO  -28.19      75.98 22.26 27.43 31.78 35.41 41.16 45.23
      50.19 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C2H4              12.52 52.47 10.2  12.72 15.02 17.0  20.14 22.54
      26.38 null
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!Here are the path reactions and their high-P limit kinetics:
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!     C2H3+C2H4O=C4H7O-14     1.4902950e+02      3.00740
1.0170800e+04
!     CH2CHCHCHOH+H=C4H7O-14  2.8500000e+13      0.00000
4.3000000e+03
!     C4H7O-14=C4H7O-13       1.3103945e+11      0.63800
3.9880000e+04
!     C4H6-13+OH=C4H7O-13     2.7100000e+12      0.00000
0.0000000e+00
!     CH2CHCHCHOH+H=C4H7O-13  1.0000000e+13      0.00000
2.9000000e+03
!     C4H7O-13=C4H7O_1_2      8.1282219e+08      1.13906
3.4790987e+04
!     CH2CHCHCHOH+H=C4H7O_1_2 3.7100000e+13      0.00000
1.0000000e+03
!     CH3CHCHCHO+H=C4H7O_1_2  2.3501400e+11      0.30815
4.9629937e+03
!     C4H7OJ(9)=C4H7O_1_2     5.6400000e+08      1.28000
2.7900000e+04
!     C2H4+C2H3O-1=C4H7OJ(9)  2.0900000e+13      0.00000
5.2000000e+03
!     CH2CHCHCHOH+H=C4H7OJ(9) 2.8500000e+13      0.00000
4.3000000e+03
!     C4H7OJ(12)=C4H7OJ(9)    2.0114313e+08      1.07833
1.8418333e+04
!     C4H7OJ(12)=C4H7O_1_2    1.5673953e+10      0.61833
2.7168333e+04

C4H7O-14(+m)=C4H7O-13(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: intra_H_migration estimate:
(Average:) Others-R2H_S    C_rad_out_H/NonDeO     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -9.788682510648208 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7813000e+00 2.3274000e+00 -5.5215000e-01 /
CHEB / 8.3277000e+00 1.5232000e+00 1.2522000e-01 /
CHEB / -3.2815000e+00 3.9372000e-01 1.0724000e-01 /
CHEB / -1.9228000e+00 -1.2714000e-01 2.7918000e-02 /
CHEB / -9.8860000e-01 -2.4980000e-01 -2.1571000e-02 /

C4H7O-14(+m)=C4H7O_1_2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -16.118073513564354
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.8673000e+00 2.6472000e+00 -1.0547000e+00 /
CHEB / 8.5183000e+00 2.6685000e+00 3.3936000e-01 /
CHEB / -3.5761000e+00 4.9021000e-01 2.1597000e-01 /
CHEB / -2.1764000e+00 -2.4342000e-01 2.5254000e-02 /
CHEB / -1.1036000e+00 -3.3299000e-01 -4.6797000e-02 /

C4H7O-13(+m)=C4H7O_1_2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: intra_H_migration estimate:
(Average:) R4H_SDS     C_rad_out_2H     Cs_H_out_H/NonDeO
      deltaHrxn(T=298K) = -6.329391002916148 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.6325000e+00 1.3420000e+00 -2.5725000e-01 /
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CHEB / 7.3541000e+00 1.6050000e+00 -8.9433000e-02 /
CHEB / -3.0203000e+00 4.6677000e-01 9.5617000e-02 /
CHEB / -1.7807000e+00 -1.3115000e-01 6.3079000e-02 /
CHEB / -8.9147000e-01 -2.5947000e-01 -1.6353000e-02 /

C4H7O-14(+m)=C4H7OJ(9)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -0.6197572944384735
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5779000e+01 5.1723000e+00 -5.0497000e-01 /
CHEB / 9.3230000e+00 1.6266000e+00 1.4197000e+00 /
CHEB / -3.1659000e+00 -3.9510000e-01 8.8464000e-02 /
CHEB / -1.8234000e+00 -5.1337000e-01 -1.4653000e-01 /
CHEB / -8.8130000e-01 -3.0759000e-01 -8.4614000e-02 /

C4H7OJ(9)(+m)=C4H7O-13(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -9.168925216209734
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0373000e+00 3.6844000e+00 -1.4150000e-01 /
CHEB / 5.8123000e+00 1.5163000e+00 9.6533000e-01 /
CHEB / -2.8504000e+00 -2.8228000e-01 7.4039000e-02 /
CHEB / -1.5695000e+00 -4.4213000e-01 -1.3317000e-01 /
CHEB / -7.2728000e-01 -2.4413000e-01 -9.2775000e-02 /

C4H7OJ(9)(+m)=C4H7O_1_2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: intra_H_migration exact:
Others-R2H_S    C_rad_out_2H     Cs_H_out_H/OneDe
      deltaHrxn(T=298K) = -15.498316219125883 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.5102000e+00 4.9594000e+00 -4.3590000e-01 /
CHEB / 3.4245000e+00 8.9080000e-01 7.1803000e-01 /
CHEB / -3.2339000e+00 -1.7096000e-01 4.8488000e-02 /
CHEB / -1.6359000e+00 -3.1034000e-01 -1.0679000e-01 /
CHEB / -7.2586000e-01 -2.0779000e-01 -7.9257000e-02 /

C2H3+C2H4O(+m)=C4H7O-14(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd_pri_rad     Cd/H2_Cd/H/Nd
      deltaHrxn(T=298K) = -34.62665248156793 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2475000e+00 9.1253000e-01 -1.7205000e-01 /
CHEB / 9.3227000e-01 1.3298000e+00 -1.3939000e-01 /
CHEB / -2.1149000e+00 6.1665000e-01 3.4413000e-02 /
CHEB / -1.4430000e+00 8.8399000e-02 7.7711000e-02 /
CHEB / -8.1116000e-01 -1.4606000e-01 3.3920000e-02 /

C2H3+C2H4O(+m)=C4H7O-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -44.415334992216145
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1217000e+00 1.8552000e+00 -6.7030000e-01 /
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CHEB / 2.1415000e+00 2.2094000e+00 1.8061000e-01 /
CHEB / -1.8009000e+00 5.6946000e-01 9.7756000e-02 /
CHEB / -1.3052000e+00 -2.2627000e-02 5.1312000e-02 /
CHEB / -7.3945000e-01 -1.6436000e-01 1.8688000e-02 /

C2H3+C2H4O(+m)=C4H7O_1_2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -50.74472599513229
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6885000e+00 2.4673000e+00 -1.1754000e+00 /
CHEB / 2.1094000e+00 3.1556000e+00 4.4890000e-01 /
CHEB / -2.1679000e+00 5.4948000e-01 1.7774000e-01 /
CHEB / -1.5375000e+00 -1.2798000e-01 3.0709000e-02 /
CHEB / -8.2884000e-01 -2.1562000e-01 -2.9508000e-03 /

C2H3+C2H4O(+m)=C4H7OJ(9)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -35.24640977600641
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.3832000e+00 5.1016000e+00 -4.8307000e-01 /
CHEB / 2.7746000e+00 1.8108000e+00 1.5011000e+00 /
CHEB / -1.7401000e+00 -3.6652000e-01 3.7653000e-02 /
CHEB / -1.1496000e+00 -3.8405000e-01 -1.1755000e-01 /
CHEB / -5.9443000e-01 -2.0208000e-01 -2.9121000e-02 /

CH2CHCHCHOH+H(+m)=C4H7O-14(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/De_Cd/H/Nd     H_rad        deltaHrxn(T=298K)
= -25.567015355631955 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0376000e+01 4.7717000e-01 -5.5701000e-02 /
CHEB / -1.1130000e+00 7.9961000e-01 -7.0130000e-02 /
CHEB / -2.0133000e+00 4.5530000e-01 1.2957000e-03 /
CHEB / -1.3392000e+00 1.1651000e-01 3.9574000e-02 /
CHEB / -7.7411000e-01 -9.2810000e-02 2.8879000e-02 /

CH2CHCHCHOH+H(+m)=C4H7O-13(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/Nd_Cd/H/De     H_rad        deltaHrxn(T=298K)
= -35.35569786628017 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0577000e+01 8.6630000e-01 -8.5206000e-02 /
CHEB / -2.5576000e+00 1.2339000e+00 -3.1753000e-02 /
CHEB / -2.1192000e+00 4.8063000e-01 6.8700000e-02 /
CHEB / -1.1795000e+00 2.5368000e-02 5.0712000e-02 /
CHEB / -6.0049000e-01 -1.0691000e-01 -6.6048000e-04 /

CH2CHCHCHOH+H(+m)=C4H7O_1_2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H/De     H_rad       deltaHrxn(T=298K) = -41.68508886919631
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.0987000e+01 1.8809000e+00 -4.4596000e-01 /
CHEB / -4.1430000e+00 1.8058000e+00 -8.8105000e-03 /
CHEB / -2.5880000e+00 5.5875000e-01 1.5264000e-01 /
CHEB / -1.3890000e+00 -3.5443000e-02 8.4225000e-02 /
CHEB / -6.6998000e-01 -1.7665000e-01 9.0113000e-05 /

CH2CHCHCHOH+H(+m)=C4H7OJ(9)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond exact:
Cd/H/De_Cd/H2     H_rad       deltaHrxn(T=298K) = -26.18677265007043
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5269000e+00 4.9124000e+00 6.2898000e-02 /
CHEB / -3.5826000e+00 2.0488000e-01 1.0242000e+00 /
CHEB / -2.2831000e+00 -3.8867000e-01 7.2944000e-02 /
CHEB / -1.0191000e+00 -2.5214000e-01 -1.1540000e-01 /
CHEB / -4.3522000e-01 -1.1326000e-01 -6.3851000e-02 /

CH2CHCHCHOH+H(+m)=C2H3+C2H4O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 9.059637125935982
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8312000e+00 -1.2304000e+00 -8.8097000e-02 /
CHEB / 6.9173000e+00 1.0660000e+00 -1.6784000e-02 /
CHEB / -1.1014000e-01 3.8209000e-01 9.4484000e-02 /
CHEB / -2.5292000e-01 -2.7317000e-02 6.7969000e-02 /
CHEB / -1.2612000e-01 -1.2493000e-01 -3.6695000e-03 /

C4H6-13+OH(+m)=C4H7O-14(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -28.017002732500746
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5579000e+00 8.4040000e-02 -3.0901000e-01 /
CHEB / 1.6665000e+00 1.7826000e+00 7.9947000e-02 /
CHEB / -2.1754000e+00 5.6796000e-01 6.8457000e-02 /
CHEB / -1.5168000e+00 1.0393000e-02 3.3952000e-02 /
CHEB / -8.3793000e-01 -1.5484000e-01 9.1776000e-03 /

C4H6-13+OH(+m)=C4H7O-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/De     O_pri_rad      deltaHrxn(T=298K)
= -37.80568524314896 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1405000e+01 6.9923000e-01 -5.0983000e-02 /
CHEB / -3.4453000e+00 1.0580000e+00 -2.6470000e-02 /
CHEB / -2.0789000e+00 4.4870000e-01 5.1767000e-02 /
CHEB / -1.2128000e+00 3.6174000e-02 4.5190000e-02 /
CHEB / -6.3041000e-01 -9.8344000e-02 2.6765000e-03 /

C4H6-13+OH(+m)=C4H7O_1_2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -44.135076246065104
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 7.5052000e+00 5.4906000e-01 -4.2436000e-01 /
CHEB / -2.3797000e+00 2.6546000e+00 4.5828000e-03 /
CHEB / -2.4246000e+00 6.2355000e-01 2.0769000e-01 /
CHEB / -1.5230000e+00 -1.0591000e-01 6.3542000e-02 /
CHEB / -7.5044000e-01 -1.9775000e-01 -3.1625000e-02 /

C4H6-13+OH(+m)=C4H7OJ(9)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -28.63676002693922
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0818000e+00 3.0340000e+00 -1.1954000e-01 /
CHEB / -1.1799000e+00 2.1018000e+00 1.0976000e+00 /
CHEB / -2.1211000e+00 -3.0107000e-01 1.2311000e-01 /
CHEB / -1.1884000e+00 -3.9527000e-01 -1.2555000e-01 /
CHEB / -5.2969000e-01 -1.7467000e-01 -7.4810000e-02 /

CH2CHCHCHOH+H(+m)=C4H6-13+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 2.4499873768687923
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1343000e+01 -9.9586000e-01 -1.1449000e-01 /
CHEB / 1.9462000e+00 1.0556000e+00 4.1001000e-02 /
CHEB / -7.5179000e-02 1.1659000e-01 1.0767000e-01 /
CHEB / -1.0996000e-01 -1.2059000e-01 8.3141000e-03 /
CHEB / -3.2297000e-02 -6.5984000e-02 -3.3483000e-02 /

CH3CHCHCHO+H(+m)=C4H7O-14(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -13.42823587070184
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.1686000e-01 -4.9003000e-01 -5.1136000e-01 /
CHEB / 6.5764000e+00 2.4246000e+00 2.6791000e-01 /
CHEB / -2.1678000e+00 5.5536000e-01 1.1670000e-01 /
CHEB / -1.5375000e+00 -7.1878000e-02 9.9984000e-03 /
CHEB / -8.2078000e-01 -1.8107000e-01 -1.0292000e-02 /

CH3CHCHCHO+H(+m)=C4H7O-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -23.216918381350048
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6647000e+00 -2.5508000e-01 -1.9891000e-01 /
CHEB / 1.9066000e+00 2.0701000e+00 3.6988000e-02 /
CHEB / -1.9418000e+00 5.7029000e-01 1.6618000e-01 /
CHEB / -1.2733000e+00 -6.7365000e-02 5.2298000e-02 /
CHEB / -6.3225000e-01 -1.6759000e-01 -3.0635000e-02 /

CH3CHCHCHO+H(+m)=C4H7O_1_2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) OCO     H_rad        deltaHrxn(T=298K) = -
29.546309384266195 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4873000e+00 1.0439000e+00 -1.6421000e-01 /
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CHEB / -1.7704000e+00 1.4359000e+00 -8.8213000e-02 /
CHEB / -2.3084000e+00 5.6977000e-01 6.9650000e-02 /
CHEB / -1.3119000e+00 2.4131000e-02 7.1215000e-02 /
CHEB / -6.5358000e-01 -1.5022000e-01 9.9612000e-03 /

CH3CHCHCHO+H(+m)=C4H7OJ(9)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -14.047993165140314
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.5546000e-01 3.3752000e+00 -1.1188000e-01 /
CHEB / 6.0231000e-01 1.3288000e+00 1.0236000e+00 /
CHEB / -2.0748000e+00 -2.0566000e-01 1.1687000e-01 /
CHEB / -1.0795000e+00 -3.5082000e-01 -1.0744000e-01 /
CHEB / -4.7061000e-01 -1.6844000e-01 -7.4470000e-02 /

CH3CHCHCHO+H(+m)=C2H3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 21.198416610866094
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2460000e+00 -1.9134000e+00 -4.2731000e-01 /
CHEB / 1.2795000e+01 1.9899000e+00 3.7885000e-01 /
CHEB / -6.9377000e-02 2.2472000e-01 1.0691000e-01 /
CHEB / -3.2603000e-01 -1.5497000e-01 8.8599000e-04 /
CHEB / -1.3451000e-01 -1.2463000e-01 -2.6596000e-02 /

CH2CHCHCHOH+H(+m)=CH3CHCHCHO+H(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -12.138779484930119
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2307000e+00 -8.7300000e-01 -1.7792000e-01 /
CHEB / -8.1111000e-01 9.2870000e-01 1.1313000e-01 /
CHEB / -4.5602000e-01 1.0510000e-01 1.0989000e-01 /
CHEB / -2.8648000e-01 -1.0932000e-01 1.1283000e-03 /
CHEB / -1.1253000e-01 -6.5226000e-02 -3.7750000e-02 /

CH3CHCHCHO+H(+m)=C4H6-13+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 14.588766861798907
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1037000e+00 -1.7871000e+00 -2.7751000e-01 /
CHEB / 6.2455000e+00 1.9416000e+00 1.6651000e-01 /
CHEB / -2.6675000e-01 1.5780000e-01 1.8653000e-01 /
CHEB / -2.6610000e-01 -2.2384000e-01 -5.6626000e-03 /
CHEB / -8.0957000e-02 -1.1728000e-01 -5.5795000e-02 /

C2H4+C2H3O-1(+m)=C4H7O-14(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -34.626652402573086
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.4045000e+00 -1.7809000e-01 -6.7883000e-01 /
CHEB / 1.9813000e+00 3.1226000e+00 3.5065000e-01 /
CHEB / -2.2637000e+00 6.1116000e-01 9.3448000e-02 /
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CHEB / -1.6768000e+00 -2.2128000e-02 2.5154000e-02 /
CHEB / -8.7872000e-01 -1.7128000e-01 1.6289000e-02 /

C2H4+C2H3O-1(+m)=C4H7O-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -44.4153349132213
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.6384000e+00 1.5792000e+00 -8.4597000e-01 /
CHEB / -1.1563000e+00 2.8812000e+00 5.7550000e-01 /
CHEB / -2.3829000e+00 4.3740000e-01 2.3072000e-01 /
CHEB / -1.3833000e+00 -1.8062000e-01 1.7533000e-02 /
CHEB / -6.6880000e-01 -1.6697000e-01 -3.2380000e-02 /

C2H4+C2H3O-1(+m)=C4H7O_1_2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -50.74472591613745
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8692000e+00 3.4922000e+00 -1.0024000e+00 /
CHEB / -3.2136000e+00 2.5671000e+00 5.8493000e-01 /
CHEB / -2.8047000e+00 3.8926000e-01 3.3651000e-01 /
CHEB / -1.5528000e+00 -2.1355000e-01 8.3060000e-02 /
CHEB / -7.3447000e-01 -2.2178000e-01 -2.0066000e-02 /

C2H4+C2H3O-1(+m)=C4H7OJ(9)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14) High-P Limit: R_Addition_MultipleBond exact:
Cd/H2_Cd/H2     Cd_pri_rad          deltaHrxn(T=298K) = -
35.246409697011565 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7684000e+00 6.2098000e+00 2.1523000e-01 /
CHEB / -4.3268000e+00 -4.1355000e-01 1.3199000e+00 /
CHEB / -2.5523000e+00 -6.3979000e-01 1.8514000e-03 /
CHEB / -1.1395000e+00 -3.4390000e-01 -1.7221000e-01 /
CHEB / -4.7431000e-01 -1.1837000e-01 -8.7576000e-02 /

C2H4+C2H3O-1(+m)=C2H3+C2H4O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 7.899484799622769E-8
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.9408000e+00 -2.0079000e+00 -4.9415000e-01 /
CHEB / 8.1818000e+00 2.1858000e+00 4.6872000e-01 /
CHEB / 2.0949000e-01 1.1674000e-01 8.9833000e-02 /
CHEB / -2.4531000e-01 -1.7834000e-01 -6.7992000e-03 /
CHEB / -1.0914000e-01 -1.1508000e-01 -3.0211000e-02 /

CH2CHCHCHOH+H(+m)=C2H4+C2H3O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 9.05963704694113
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9959000e+00 -3.8384000e-01 -1.6718000e-01 /
CHEB / 4.0321000e+00 4.2794000e-01 1.6957000e-01 /
CHEB / -1.5128000e-03 1.2406000e-02 2.5381000e-02 /
CHEB / -8.8567000e-02 -3.9415000e-02 -1.4135000e-02 /
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CHEB / -2.8009000e-02 -2.0295000e-02 -1.2378000e-02 /

C4H6-13+OH(+m)=C2H4+C2H3O-1(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 6.60964967007234
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0634000e+00 -1.4177000e+00 -5.2497000e-01 /
CHEB / 5.4978000e+00 1.7047000e+00 5.4937000e-01 /
CHEB / -1.7962000e-01 -9.5936000e-02 8.1472000e-02 /
CHEB / -2.4203000e-01 -1.8202000e-01 -7.5411000e-02 /
CHEB / -9.0687000e-02 -3.9127000e-02 -4.2589000e-02 /

CH3CHCHCHO+H(+m)=C2H4+C2H3O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 21.198416531871246
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3540000e+00 -8.9760000e-01 -3.6715000e-01 /
CHEB / 8.3227000e+00 1.0526000e+00 3.8131000e-01 /
CHEB / -1.6931000e-01 -1.7803000e-02 6.0788000e-02 /
CHEB / -1.9860000e-01 -1.2382000e-01 -5.1370000e-02 /
CHEB / -5.8773000e-02 -3.5501000e-02 -3.2073000e-02 /

C4H7O-14(+m)=C4H7OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -13.718374499925785
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.2762000e+00 -5.3384000e-01 -5.2464000e-01 /
CHEB / 1.1856000e+01 2.3372000e+00 2.7704000e-01 /
CHEB / -2.0791000e+00 5.5603000e-01 1.1217000e-01 /
CHEB / -1.5055000e+00 -6.1862000e-02 2.6056000e-03 /
CHEB / -8.1378000e-01 -1.7221000e-01 -1.4366000e-02 /

C4H7O-13(+m)=C4H7OJ(12)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -3.929691989277577
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.2463000e+00 -4.3583000e-01 -1.7012000e-01 /
CHEB / 1.0286000e+01 1.9335000e+00 3.4641000e-02 /
CHEB / -1.8104000e+00 5.9775000e-01 1.5705000e-01 /
CHEB / -1.2557000e+00 -3.9378000e-02 6.2004000e-02 /
CHEB / -6.5160000e-01 -1.6127000e-01 -2.5166000e-02 /

C4H7O_1_2(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = 2.399699013638571
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.5499000e-01 6.3504000e-01 -4.2444000e-02 /
CHEB / 7.2564000e+00 1.0245000e+00 -3.3142000e-02 /
CHEB / -2.0398000e+00 5.1098000e-01 4.3456000e-02 /
CHEB / -1.2913000e+00 8.0960000e-02 5.8852000e-02 /
CHEB / -6.8252000e-01 -1.1248000e-01 1.9289000e-02 /
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C4H7OJ(9)(+m)=C4H7OJ(12)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -13.098617205487312
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1187000e+00 1.3237000e+00 -2.2124000e-01 /
CHEB / 6.4538000e-01 6.1864000e-01 1.7014000e-01 /
CHEB / -2.0285000e+00 8.7638000e-02 6.4171000e-02 /
CHEB / -9.6788000e-01 -4.0306000e-02 -1.0655000e-02 /
CHEB / -4.2796000e-01 -3.3681000e-02 -1.9763000e-02 /

C2H3+C2H4O(+m)=C4H7OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -48.34502698149372
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.5172000e+00 -1.9083000e+00 -4.3178000e-01 /
CHEB / 6.6681000e+00 1.9649000e+00 3.8782000e-01 /
CHEB / 5.2977000e-02 2.4408000e-01 1.0308000e-01 /
CHEB / -3.3214000e-01 -1.4165000e-01 6.9335000e-04 /
CHEB / -1.6470000e-01 -1.2437000e-01 -2.4392000e-02 /

CH2CHCHCHOH+H(+m)=C4H7OJ(12)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -39.28538985555774
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3022000e+01 -8.2203000e-01 -1.5770000e-01 /
CHEB / 4.9072000e-01 8.9361000e-01 1.1066000e-01 /
CHEB / -1.2643000e-01 6.9076000e-02 7.9009000e-02 /
CHEB / -1.3094000e-01 -9.8072000e-02 5.3773000e-03 /
CHEB / -5.6084000e-02 -4.9731000e-02 -2.4161000e-02 /

C4H6-13+OH(+m)=C4H7OJ(12)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -41.73537723242653
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3402000e+00 -1.8637000e+00 -2.6881000e-01 /
CHEB / 1.8703000e+00 1.9740000e+00 1.4672000e-01 /
CHEB / -2.6875000e-01 2.2097000e-01 1.9101000e-01 /
CHEB / -3.1454000e-01 -2.1463000e-01 6.6549000e-03 /
CHEB / -1.2130000e-01 -1.3486000e-01 -5.3908000e-02 /

C2H4+C2H3O-1(+m)=C4H7OJ(12)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (C4H7O-14)     deltaHrxn(T=298K) = -48.34502690249887
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1808000e+01 -1.4059000e-01 -9.6962000e-02 /
CHEB / 6.4636000e-01 1.9582000e-01 1.2978000e-01 /
CHEB / -3.0853000e-01 -3.9632000e-02 -1.7657000e-02 /
CHEB / -1.4630000e-01 -2.4558000e-02 -2.0588000e-02 /
CHEB / -5.4697000e-02 2.3404000e-03 -5.3969000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
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!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHCCHOH  31.65 76.38 23.26 28.14 31.96 34.91 39.19 42.25 47.88
      null
!     CHCHCHCHOH  43.05 77.06 22.88 28.15 32.11 35.0  39.07 41.93 46.52
      null
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!     CH2CHCHCOH  43.05 77.06 22.88 28.15 32.11 35.0  39.07 41.93 46.52
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H4              68.17 65.12 17.41 21.68 24.25 27.71 31.23 33.72
      37.82 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C2H2              53.86 48.02 10.56 11.98 12.98 13.74 14.94 15.92
      17.7  null
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     CHCCHCHOH   26.04 72.81 21.36 26.28 29.2  32.79 36.28 38.62 42.53
      null
!Here are the path reactions and their high-P limit kinetics:
!     C4H4+OH=CH2CHCCHOH      7.6000000e+07      1.70000
1.0000000e+03
!     CHCHCHCHOH=CH2CHCCHOH   2.0320555e+08      1.13906
3.4790987e+04
!     C2H2+C2H3O-1=CHCHCHCHOH 1.2550000e+05      1.90000
2.1100000e+03
!     CHCCHCHOH+H=CHCHCHCHOH  2.2500000e+13      0.00000
5.4000000e+03
!     CH2CHCHCHO=CHCHCHCHOH   8.1282219e+08      1.13906
3.4790987e+04
!     CHCHCHCHOH=CH2CHCHCOH   2.0320555e+08      1.13906
3.4790987e+04
!     CH2CHCHCOH=CH2CHCCHOH   1.9697990e+11      0.77000
4.5050000e+04
!     CH2CHCHCHO=CH2CHCCHOH   2.0320555e+08      1.13906
3.4790987e+04

CHCHCHCHOH(+m)=CH2CHCCHOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) High-P Limit: intra_H_migration estimate:
(Average:) R3H_DS     Cd_rad_out_singleH     Cd_H_out_doubleC
      deltaHrxn(T=298K) = -11.398915862129016 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9777000e+01 9.0601000e+00 -1.9568000e-01 /
CHEB / 4.7968000e+00 -7.2454000e-01 1.0172000e+00 /
CHEB / -2.5765000e+00 -7.1692000e-01 1.4172000e-01 /
CHEB / -1.0694000e+00 -3.2596000e-01 -7.5308000e-02 /
CHEB / -4.6375000e-01 -9.8579000e-02 -4.6043000e-02 /

C4H4+OH(+m)=CH2CHCCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) High-P Limit: R_Addition_MultipleBond
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estimate: (Average:) Ct/H_Ct/De     O_pri_rad         deltaHrxn(T=298K)
= -45.835129813213904 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.8634000e+00 7.4106000e+00 -3.1559000e-01 /
CHEB / -4.6570000e+00 -8.3386000e-02 1.6176000e+00 /
CHEB / -2.1493000e+00 -7.8844000e-01 1.6530000e-01 /
CHEB / -9.5750000e-01 -4.6153000e-01 -1.3761000e-01 /
CHEB / -4.1791000e-01 -1.5530000e-01 -7.9029000e-02 /

C4H4+OH(+m)=CHCHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -34.43621395108489
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.6598000e+00 2.4956000e+00 3.6749000e-01 /
CHEB / -2.0695000e+00 -8.4760000e-02 -1.1653000e-01 /
CHEB / -1.4472000e+00 -9.0057000e-02 -3.9474000e-02 /
CHEB / -7.2328000e-01 -5.7605000e-02 -2.9320000e-02 /
CHEB / -3.4610000e-01 -3.4801000e-02 -2.3943000e-02 /

C2H2+C2H3O-1(+m)=CH2CHCCHOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -51.69458068626604
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.2016000e+00 8.6736000e+00 5.7776000e-03 /
CHEB / -4.1387000e+00 -3.0038000e-01 1.8587000e+00 /
CHEB / -2.1048000e+00 -1.0362000e+00 6.4946000e-02 /
CHEB / -9.7659000e-01 -5.5943000e-01 -1.9952000e-01 /
CHEB / -4.3287000e-01 -1.7204000e-01 -9.9413000e-02 /

C2H2+C2H3O-1(+m)=CHCHCHCHOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) High-P Limit: R_Addition_MultipleBond
exact:  Ct/H_Ct/H     Cd_pri_rad          deltaHrxn(T=298K) = -
40.29566482413703 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1645000e+00 2.7733000e+00 5.4484000e-01 /
CHEB / -3.4714000e+00 -6.5099000e-01 -4.4823000e-01 /
CHEB / -1.5829000e+00 -4.2914000e-02 -4.7777000e-02 /
CHEB / -6.7749000e-01 1.9331000e-02 1.5032000e-02 /
CHEB / -3.2345000e-01 -3.5321000e-03 1.8133000e-03 /

C4H4+OH(+m)=C2H2+C2H3O-1(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = 5.859450873052143
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2292000e+00 -2.4050000e-01 -1.3191000e-01 /
CHEB / 5.8371000e+00 3.1442000e-01 1.6523000e-01 /
CHEB / 7.1680000e-01 -4.9718000e-02 -1.4532000e-02 /
CHEB / 1.1525000e-01 -3.2550000e-02 -2.2361000e-02 /
CHEB / 1.8958000e-02 1.3403000e-03 -1.6040000e-03 /
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CHCCHCHOH+H(+m)=CH2CHCCHOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -43.3851424285777
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.7774000e+00 8.2906000e+00 -7.2244000e-02 /
CHEB / -3.2812000e+00 -9.4833000e-02 1.8251000e+00 /
CHEB / -2.2664000e+00 -9.8801000e-01 1.0076000e-01 /
CHEB / -1.0187000e+00 -5.5193000e-01 -1.9104000e-01 /
CHEB / -4.3772000e-01 -1.7470000e-01 -9.8309000e-02 /

CHCCHCHOH+H(+m)=CHCHCHCHOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) High-P Limit: R_Addition_MultipleBond
exact:  Ct/De_Ct/H     H_rad        deltaHrxn(T=298K) = -
31.986226566448686 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1364000e+00 2.7042000e+00 4.9078000e-01 /
CHEB / -2.8566000e+00 -5.8672000e-01 -3.9890000e-01 /
CHEB / -1.7891000e+00 -4.2822000e-02 -4.5385000e-02 /
CHEB / -7.2812000e-01 1.5260000e-02 1.1642000e-02 /
CHEB / -3.3042000e-01 -3.6947000e-03 1.3629000e-03 /

CHCCHCHOH+H(+m)=C4H4+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = 2.449987384636197
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6885000e+00 -2.5345000e-01 -1.3680000e-01 /
CHEB / 4.9597000e+00 3.2936000e-01 1.6975000e-01 /
CHEB / 5.7010000e-01 -4.9594000e-02 -1.2794000e-02 /
CHEB / 8.3494000e-02 -3.4300000e-02 -2.3207000e-02 /
CHEB / 2.1515000e-02 5.3030000e-04 -2.3814000e-03 /

CHCCHCHOH+H(+m)=C2H2+C2H3O-1(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = 8.309438257688345
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1240000e+00 -1.1335000e-02 -7.8136000e-03 /
CHEB / 4.4950000e+00 1.4694000e-02 1.0110000e-02 /
CHEB / 5.7767000e-01 -2.6737000e-03 -1.8119000e-03 /
CHEB / 1.6901000e-01 -9.0772000e-04 -6.3736000e-04 /
CHEB / 3.8660000e-02 1.1330000e-04 7.5448000e-05 /

CH2CHCCHOH(+m)=CH2CHCHCHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -23.737452521033937
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5843000e+00 9.0651000e-01 -1.1919000e-01 /
CHEB / 1.5624000e+00 9.4301000e-01 6.2026000e-02 /
CHEB / -1.7207000e+00 2.2391000e-01 8.5862000e-02 /
CHEB / -8.5289000e-01 -5.9806000e-02 1.0732000e-02 /
CHEB / -4.0135000e-01 -7.5296000e-02 -2.6406000e-02 /
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CHCHCHCHOH(+m)=CH2CHCHCHO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -35.13636838316295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6094000e+00 1.9831000e+00 -1.1615000e-02 /
CHEB / 6.2849000e-01 1.7495000e-02 1.1980000e-02 /
CHEB / -1.8480000e+00 -2.0643000e-04 -1.1450000e-04 /
CHEB / -7.9095000e-01 -8.4458000e-04 -5.8214000e-04 /
CHEB / -3.5126000e-01 -1.8977000e-04 -1.3151000e-04 /

C4H4+OH(+m)=CH2CHCHCHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -69.57258233424784
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2506000e+01 -1.4267000e-01 -9.7734000e-02 /
CHEB / 3.8879000e-01 1.9338000e-01 1.2753000e-01 /
CHEB / -1.3373000e-01 -3.4836000e-02 -1.4753000e-02 /
CHEB / -1.3071000e-01 -2.1896000e-02 -1.8460000e-02 /
CHEB / -7.7803000e-02 1.2155000e-05 -1.9423000e-03 /

C2H2+C2H3O-1(+m)=CH2CHCHCHO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -75.43203320729998
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0640000e+01 -3.3604000e-06 -2.3544000e-06 /
CHEB / 7.1452000e-01 7.8662000e-06 5.4723000e-06 /
CHEB / 2.0588000e-01 8.5227000e-07 6.1987000e-07 /
CHEB / 8.1185000e-02 -8.8710000e-07 -6.1169000e-07 /
CHEB / 2.4864000e-02 -1.1674000e-06 -8.2767000e-07 /

CHCCHCHOH+H(+m)=CH2CHCHCHO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -67.12259494961164
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1815000e+01 -3.6715000e-06 -2.5687000e-06 /
CHEB / 1.2969000e+00 7.5141000e-06 5.2346000e-06 /
CHEB / 2.4102000e-03 7.9886000e-07 5.6579000e-07 /
CHEB / 3.4381000e-02 -6.6417000e-07 -4.5312000e-07 /
CHEB / 1.9027000e-02 -9.8272000e-07 -6.9258000e-07 /

CH2CHCCHOH(+m)=CH2CHCHCOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = 11.398915862129016
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9529000e+01 8.6971000e+00 1.7157000e-02 /
CHEB / 1.2792000e+01 -4.3280000e-01 1.7334000e+00 /
CHEB / -2.2953000e+00 -1.1531000e+00 8.7378000e-02 /
CHEB / -1.1008000e+00 -4.5208000e-01 -2.0811000e-01 /
CHEB / -4.4620000e-01 -1.8278000e-01 -7.8304000e-02 /

CHCHCHCHOH(+m)=CH2CHCHCOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) High-P Limit: intra_H_migration estimate:
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(Average:) R4H_DSD     Cd_rad_out_singleH     Cd_H_out_singleNd
      deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3144000e+01 2.5633000e+00 3.8263000e-01 /
CHEB / 7.4602000e+00 -4.5821000e-01 -3.0192000e-01 /
CHEB / -1.6802000e+00 -4.2704000e-02 -4.0476000e-02 /
CHEB / -7.3892000e-01 7.8062000e-03 5.5492000e-03 /
CHEB / -3.4561000e-01 -2.6966000e-03 1.0710000e-03 /

C4H4+OH(+m)=CH2CHCHCOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -34.43621395108489
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7643000e+00 -2.3628000e-01 -1.2838000e-01 /
CHEB / 4.7109000e+00 2.9805000e-01 1.5430000e-01 /
CHEB / 3.5937000e-01 -3.3872000e-02 -5.7193000e-03 /
CHEB / 4.7113000e-02 -3.1899000e-02 -2.0769000e-02 /
CHEB / 1.3738000e-02 -2.9171000e-03 -4.2059000e-03 /

C2H2+C2H3O-1(+m)=CH2CHCHCOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -40.29566482413703
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0549000e+00 -9.9041000e-03 -6.8404000e-03 /
CHEB / 2.7210000e+00 1.2674000e-02 8.7408000e-03 /
CHEB / 8.0282000e-01 -2.0855000e-03 -1.4194000e-03 /
CHEB / 2.4596000e-01 -8.4760000e-04 -5.9277000e-04 /
CHEB / 6.1747000e-02 5.4541000e-05 3.5676000e-05 /

CHCCHCHOH+H(+m)=CH2CHCHCOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #189 (CH2CHCCHOH) deltaHrxn(T=298K) = -31.986226566448686
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.9600000e+00 -1.0628000e-02 -7.3331000e-03 /
CHEB / 3.5320000e+00 1.3736000e-02 9.4615000e-03 /
CHEB / 6.1989000e-01 -2.4404000e-03 -1.6576000e-03 /
CHEB / 1.9556000e-01 -8.6490000e-04 -6.0663000e-04 /
CHEB / 5.3128000e-02 8.7101000e-05 5.7968000e-05 /

!PDepNetwork CH2CHCHCHOH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHCHCHOH -16.05      75.67 23.07 28.9  33.47 36.92 41.89 45.42
      51.05 null
!     CHCHCHCHOH  43.05 77.06 22.88 28.15 32.11 35.0  39.07 41.93 46.52
      null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
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!     C2H3O-1           32.17 62.75 14.65 17.72 20.0  21.59 23.58 24.88
      27.02
!     CH2CHCCHOH  38.05 76.08 23.22 28.44 32.51 35.55 39.78 42.75 47.48
!MRH CBS-QB3 w/1DHR corrections
!     nC4H5             85.18 69.37 18.93 23.55 27.16 29.92 34.02 37.03
      41.81 null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2CHCHCOH  43.05 77.06 22.88 28.15 32.11 35.0  39.07 41.93 46.52
      null
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!Here are the path reactions and their high-P limit kinetics:
!     CHCHCHCHOH+H=CH2CHCHCHOH      5.3600000e+14      0.00000
9.8000000e+02
!     C2H3+C2H3O-1=CH2CHCHCHOH      7.2300000e+13      0.00000
0.0000000e+00
!     CH2CHCCHOH+H=CH2CHCHCHOH      1.4157154e+13      -0.15000
2.9166667e+02
!     nC4H5+OH=CH2CHCHCHOH    1.4157154e+13      -0.15000
2.9166667e+02
!     CH2CHCHCOH+H=CH2CHCHCHOH      1.4157154e+13      -0.15000
2.9166667e+02
!     CH2CHCHCHO+H=CH2CHCHCHOH      1.4157154e+13      -0.15000
2.9166667e+02

CHCHCHCHOH+H(+m)=CH2CHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination exact:
Cd_pri_rad     H_rad          deltaHrxn(T=298K) = -111.18808665979387
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3980000e+01 4.8658000e-01 -9.2782000e-02 /
CHEB / -7.0681000e-01 7.8277000e-01 -1.0498000e-01 /
CHEB / -6.3679000e-01 4.5026000e-01 -2.2095000e-03 /
CHEB / -3.4026000e-01 1.6416000e-01 4.9386000e-02 /
CHEB / -1.5503000e-01 2.1501000e-03 4.5771000e-02 /

C2H3+C2H3O-1(+m)=CH2CHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination exact:
Cd_pri_rad     Cd_pri_rad           deltaHrxn(T=298K) = -
120.40757496095215 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3294000e+01 6.0465000e-01 -1.2221000e-01 /
CHEB / -1.1532000e+00 8.5134000e-01 -7.7676000e-02 /
CHEB / -7.1002000e-01 4.1409000e-01 4.2841000e-02 /
CHEB / -3.6086000e-01 1.1140000e-01 6.7770000e-02 /
CHEB / -1.5627000e-01 -2.5888000e-02 3.8058000e-02 /

CHCHCHCHOH+H(+m)=C2H3+C2H3O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 9.219488301158272
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1443000e+00 -1.2398000e+00 -1.1543000e-01 /
CHEB / 5.5085000e+00 1.0038000e+00 -2.4522000e-02 /
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CHEB / 3.7683000e-01 3.7139000e-01 9.5989000e-02 /
CHEB / -1.2115000e-01 8.5070000e-03 7.3903000e-02 /
CHEB / -1.4543000e-01 -8.9372000e-02 9.6690000e-03 /

CH2CHCCHOH+H(+m)=CH2CHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/OneDe     H_rad         deltaHrxn(T=298K) = -
106.18853248274705 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2377000e+01 4.2416000e-01 -7.9605000e-02 /
CHEB / -9.4094000e-01 7.2030000e-01 -1.0964000e-01 /
CHEB / -6.0688000e-01 4.5499000e-01 -2.6367000e-02 /
CHEB / -3.4101000e-01 1.9608000e-01 3.0734000e-02 /
CHEB / -1.6433000e-01 2.7398000e-02 4.3019000e-02 /

CHCHCHCHOH+H(+m)=CH2CHCCHOH+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -4.999554177046825
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4650000e+00 -1.3427000e+00 -8.9932000e-02 /
CHEB / 3.5491000e+00 9.8460000e-01 -5.9679000e-02 /
CHEB / 6.3836000e-01 4.4177000e-01 6.6003000e-02 /
CHEB / -7.6557000e-02 6.1798000e-02 8.2666000e-02 /
CHEB / -1.5161000e-01 -7.7574000e-02 3.1666000e-02 /

CH2CHCCHOH+H(+m)=C2H3+C2H3O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 14.21904247820509
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0385000e+00 -1.2620000e+00 -1.1338000e-01 /
CHEB / 6.7131000e+00 9.9209000e-01 -3.0893000e-02 /
CHEB / 2.5516000e-01 3.8830000e-01 8.9836000e-02 /
CHEB / -1.4707000e-01 2.5229000e-02 7.6353000e-02 /
CHEB / -1.6051000e-01 -8.4379000e-02 1.5569000e-02 /

nC4H5+OH(+m)=CH2CHCHCHOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     O_pri_rad       deltaHrxn(T=298K) = -
109.90848338015522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2259000e+01 4.7451000e-01 -9.0078000e-02 /
CHEB / -9.9220000e-01 7.7221000e-01 -1.0646000e-01 /
CHEB / -6.5681000e-01 4.5231000e-01 -7.0586000e-03 /
CHEB / -3.5538000e-01 1.7030000e-01 4.6233000e-02 /
CHEB / -1.6864000e-01 6.3623000e-03 4.5750000e-02 /

CHCHCHCHOH+H(+m)=nC4H5+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -1.2796032796386463
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4130000e+00 -1.3186000e+00 -9.4151000e-02 /
CHEB / 3.4295000e+00 9.9732000e-01 -5.3452000e-02 /
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CHEB / 4.7204000e-01 4.2466000e-01 7.4959000e-02 /
CHEB / -1.4618000e-01 4.4810000e-02 8.2298000e-02 /
CHEB / -1.7198000e-01 -8.2744000e-02 2.5780000e-02 /

nC4H5+OH(+m)=C2H3+C2H3O-1(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 10.499091580796922
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.1603000e+00 -1.2443000e+00 -1.1493000e-01 /
CHEB / 5.4733000e+00 1.0018000e+00 -2.5832000e-02 /
CHEB / 3.3024000e-01 3.7493000e-01 9.4786000e-02 /
CHEB / -1.4019000e-01 1.1686000e-02 7.4471000e-02 /
CHEB / -1.6032000e-01 -8.8563000e-02 1.0842000e-02 /

CH2CHCCHOH+H(+m)=nC4H5+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 3.7199508974081716
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6402000e+00 -1.3501000e+00 -8.8078000e-02 /
CHEB / 4.2474000e+00 9.8205000e-01 -6.1814000e-02 /
CHEB / 4.2771000e-01 4.4675000e-01 6.3289000e-02 /
CHEB / -1.6354000e-01 6.6149000e-02 8.2749000e-02 /
CHEB / -1.8869000e-01 -7.6408000e-02 3.3270000e-02 /

CH2CHCHCOH+H(+m)=CH2CHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
111.18808665979387 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2211000e+01 4.8050000e-01 -9.1411000e-02 /
CHEB / -9.5197000e-01 7.7754000e-01 -1.0576000e-01 /
CHEB / -6.5039000e-01 4.5135000e-01 -4.6558000e-03 /
CHEB / -3.4558000e-01 1.6724000e-01 4.7828000e-02 /
CHEB / -1.5775000e-01 4.2325000e-03 4.5788000e-02 /

CHCHCHCHOH+H(+m)=CH2CHCHCOH+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 0.0 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5173000e+00 -1.3155000e+00 -9.4831000e-02 /
CHEB / 4.1480000e+00 9.9843000e-01 -5.2506000e-02 /
CHEB / 6.3757000e-01 4.2247000e-01 7.6009000e-02 /
CHEB / -8.7009000e-02 4.2876000e-02 8.2143000e-02 /
CHEB / -1.4821000e-01 -8.3249000e-02 2.5048000e-02 /

CH2CHCHCOH+H(+m)=C2H3+C2H3O-1(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = 9.219488301158272
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2446000e+00 -1.2421000e+00 -1.1517000e-01 /
CHEB / 5.3877000e+00 1.0028000e+00 -2.5187000e-02 /
CHEB / 3.5002000e-01 3.7319000e-01 9.5382000e-02 /
CHEB / -1.2840000e-01 1.0103000e-02 7.4195000e-02 /
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CHEB / -1.4881000e-01 -8.8974000e-02 1.0261000e-02 /

CH2CHCHCOH+H(+m)=CH2CHCCHOH+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -4.999554177046825
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.6182000e+00 -1.3465000e+00 -8.8984000e-02 /
CHEB / 3.3635000e+00 9.8335000e-01 -6.0772000e-02 /
CHEB / 6.2797000e-01 4.4430000e-01 6.4638000e-02 /
CHEB / -8.4012000e-02 6.3976000e-02 8.2722000e-02 /
CHEB / -1.5531000e-01 -7.7001000e-02 3.2478000e-02 /

CH2CHCHCOH+H(+m)=nC4H5+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -1.2796032796386463
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.5475000e+00 -1.3219000e+00 -9.3421000e-02 /
CHEB / 3.2676000e+00 9.9615000e-01 -5.4409000e-02 /
CHEB / 4.5476000e-01 4.2703000e-01 7.3807000e-02 /
CHEB / -1.5295000e-01 4.6783000e-02 8.2465000e-02 /
CHEB / -1.7570000e-01 -8.2251000e-02 2.6548000e-02 /

CH2CHCHCHO+H(+m)=CH2CHCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     H_rad          deltaHrxn(T=298K) = -
76.05171827663092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2471000e+01 2.0207000e-01 -3.9904000e-02 /
CHEB / -3.7012000e-01 3.7807000e-01 -7.2002000e-02 /
CHEB / -3.2455000e-01 3.0799000e-01 -5.1588000e-02 /
CHEB / -2.2671000e-01 2.1466000e-01 -2.6010000e-02 /
CHEB / -1.4867000e-01 1.2282000e-01 -3.5013000e-03 /

CHCHCHCHOH+H(+m)=CH2CHCHCHO+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -35.13636838316295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2586000e+01 -1.4259000e+00 -8.5623000e-02 /
CHEB / 1.4865000e+00 9.0424000e-01 -7.8588000e-02 /
CHEB / 1.5086000e-01 4.7577000e-01 3.3138000e-02 /
CHEB / -1.5881000e-01 1.2921000e-01 7.2306000e-02 /
CHEB / -1.7954000e-01 -3.9869000e-02 4.6204000e-02 /

C2H3+C2H3O-1(+m)=CH2CHCHCHO+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -44.35585668432123
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2384000e+01 -1.3264000e+00 -1.1361000e-01 /
CHEB / 8.2005000e-01 9.3683000e-01 -5.0417000e-02 /
CHEB / 9.0519000e-03 4.2046000e-01 6.9661000e-02 /
CHEB / -1.8642000e-01 7.7814000e-02 7.7480000e-02 /
CHEB / -1.7253000e-01 -5.7001000e-02 3.0874000e-02 /
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CH2CHCCHOH+H(+m)=CH2CHCHCHO+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -30.136814206116135
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0618000e+01 -1.4748000e+00 -7.4126000e-02 /
CHEB / 1.4376000e+00 8.6887000e-01 -8.6201000e-02 /
CHEB / 2.3425000e-01 4.9826000e-01 1.1611000e-02 /
CHEB / -1.5496000e-01 1.6299000e-01 6.1985000e-02 /
CHEB / -1.9326000e-01 -2.3450000e-02 5.1014000e-02 /

nC4H5+OH(+m)=CH2CHCHCHO+H(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -33.8567651035243
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0802000e+01 -1.4356000e+00 -8.3173000e-02 /
CHEB / 1.2319000e+00 8.9840000e-01 -8.0465000e-02 /
CHEB / 1.4003000e-01 4.8071000e-01 2.8975000e-02 /
CHEB / -1.7300000e-01 1.3544000e-01 7.0749000e-02 /
CHEB / -1.9396000e-01 -3.7207000e-02 4.7425000e-02 /

CH2CHCHCOH+H(+m)=CH2CHCHCHO+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CH2CHCHCHOH)  deltaHrxn(T=298K) = -35.13636838316295
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0786000e+01 -1.4308000e+00 -8.4376000e-02 /
CHEB / 1.2566000e+00 9.0136000e-01 -7.9558000e-02 /
CHEB / 1.4182000e-01 4.7829000e-01 3.1046000e-02 /
CHEB / -1.6366000e-01 1.3232000e-01 7.1549000e-02 /
CHEB / -1.8266000e-01 -3.8556000e-02 4.6833000e-02 /

!PDepNetwork CHCCHCHOH
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CHCCHCHOH   28.19 73.91 22.23 26.36 29.54 32.03 35.69 38.3  42.41
!MRH CBS-QB3 w/1DHR corrections
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H              137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     C2H3O-1          32.17 62.75 14.65 17.72 20.0  21.59 23.58 24.88
      27.02
!     CHCCCHOH    75.69 76.2  21.5  25.07 27.73 29.93 32.81 34.84 38.89
      null
!     nC4H3            132.99      67.35 17.24 20.41 22.8  24.66 27.47
      29.56 32.87
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     C2H+C2H3O-1=CHCCHCHOH   1.0000000e+14      0.00000
0.0000000e+00
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!     CHCCCHOH+H=CHCCHCHOH    1.4157154e+13      -0.15000
2.9166667e+02
!     nC4H3+OH=CHCCHCHOH      1.4157154e+13      -0.15000
2.9166667e+02

C2H+C2H3O-1(+m)=CHCCHCHOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH) High-P Limit: R_Recombination exact:  Ct_rad
Cd_pri_rad        deltaHrxn(T=298K) = -141.105395855619 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3196000e+00 9.2238000e+00 -1.1769000e+00 /
CHEB / -4.1506000e+00 1.4267000e+00 9.3259000e-01 /
CHEB / -1.9295000e+00 2.8235000e-01 2.9556000e-01 /
CHEB / -8.9684000e-01 2.3793000e-02 7.1235000e-02 /
CHEB / -4.2851000e-01 -1.2441000e-02 1.1758000e-02 /

CHCCCHOH+H(+m)=CHCCHCHOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/OneDe     H_rad         deltaHrxn(T=298K) = -
99.58936103516328 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1277000e+01 1.5685000e+00 -4.6082000e-01 /
CHEB / -2.1743000e+00 1.7344000e+00 -1.9607000e-01 /
CHEB / -1.3025000e+00 7.7890000e-01 5.7911000e-02 /
CHEB / -7.2165000e-01 2.7304000e-01 8.4188000e-02 /
CHEB / -3.9535000e-01 6.9138000e-02 4.5049000e-02 /

C2H+C2H3O-1(+m)=CHCCCHOH+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH)    deltaHrxn(T=298K) = -41.51603482045574
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2321000e+01 -2.0117000e-01 -1.2337000e-01 /
CHEB / 5.0503000e-01 2.2484000e-01 1.3215000e-01 /
CHEB / 1.8372000e-01 5.3018000e-03 1.0908000e-02 /
CHEB / 6.9866000e-02 -2.2603000e-02 -1.3849000e-02 /
CHEB / 1.6318000e-02 -9.5776000e-03 -7.7055000e-03 /

nC4H3+OH(+m)=CHCCHCHOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     O_pri_rad       deltaHrxn(T=298K) = -
113.47827156179201 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2296000e+00 3.9878000e+00 -1.1988000e+00 /
CHEB / -2.9392000e+00 2.0707000e+00 1.7445000e-01 /
CHEB / -1.5881000e+00 6.8550000e-01 2.1898000e-01 /
CHEB / -8.0933000e-01 1.8203000e-01 1.0558000e-01 /
CHEB / -4.1937000e-01 2.9425000e-02 3.2466000e-02 /

C2H+C2H3O-1(+m)=nC4H3+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH)    deltaHrxn(T=298K) = -27.627124293827006
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2279000e+01 -2.3440000e-01 -1.3475000e-01 /
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CHEB / 2.8879000e-01 2.6200000e-01 1.4345000e-01 /
CHEB / 1.9351000e-01 6.3720000e-03 1.2985000e-02 /
CHEB / 6.3473000e-02 -2.6910000e-02 -1.5227000e-02 /
CHEB / 4.1834000e-03 -1.0970000e-02 -8.4812000e-03 /

nC4H3+OH(+m)=CHCCCHOH+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CHCCHCHOH)    deltaHrxn(T=298K) = -13.888910526628742
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.6063000e+00 -6.6842000e-01 -2.2759000e-01 /
CHEB / 1.5067000e+00 6.6976000e-01 1.7965000e-01 /
CHEB / 4.1673000e-01 9.9161000e-02 8.2954000e-02 /
CHEB / 8.2202000e-02 -5.2652000e-02 -2.2523000e-03 /
CHEB / -1.9471000e-03 -4.4211000e-02 -2.2787000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3CHCHCO   2.71  74.59 22.07 26.58 30.19 33.2  37.95 41.34 45.58
      null
!     CH3CCHCHO   28.71 77.79 21.92 26.22 29.84 32.89 37.82 41.32 45.43
      null
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     CH3CCHCHO=CH3CHCHCO     2.0320555e+08      1.13906
3.4790987e+04
!     CH2CHCHCHO=CH3CHCHCO    2.0320555e+08      1.13906
3.4790987e+04
!     pC3H5+CO=CH3CHCHCO      1.5100000e+11      0.00000
4.8100000e+03

pC3H5+CO(+m)=CH3CHCHCO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #803 (CH3CHCHCO) High-P Limit: R_Addition_COm exact:
Cd_pri_rad     COm      deltaHrxn(T=298K) = -34.616416157236856 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7283000e+00 6.9501000e-01 -9.9391000e-02 /
CHEB / 1.9144000e-01 8.6541000e-01 -2.4882000e-02 /
CHEB / -6.3277000e-01 3.3600000e-01 3.8931000e-02 /
CHEB / -2.3327000e-01 5.3970000e-02 3.3673000e-02 /
CHEB / -5.7730000e-02 -2.1191000e-02 9.2867000e-03 /
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CH3CHCHCO(+m)=CH2CHCHCHO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #803 (CH3CHCHCO)  deltaHrxn(T=298K) = 5.199565652565774
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -5.8177000e+00 6.9501000e-01 -9.9391000e-02 /
CHEB / 1.3027000e+01 8.6541000e-01 -2.4882000e-02 /
CHEB / -4.4153000e-01 3.3600000e-01 3.8931000e-02 /
CHEB / -1.8721000e-01 5.3970000e-02 3.3673000e-02 /
CHEB / -4.4933000e-02 -2.1191000e-02 9.2867000e-03 /

CH3CHCHCO(+m)=CH3CCHCHO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #803 (CH3CHCHCO)  deltaHrxn(T=298K) = 25.997379160316257
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5006000e+01 1.8810000e+00 -7.5445000e-02 /
CHEB / 2.0252000e+01 8.2890000e-02 5.2002000e-02 /
CHEB / -2.6635000e-01 3.6150000e-02 2.2102000e-02 /
CHEB / -4.8899000e-02 -7.8491000e-03 -4.2202000e-03 /
CHEB / 1.8150000e-02 -8.7184000e-03 -5.0969000e-03 /

pC3H5+CO(+m)=CH3CCHCHO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #803 (CH3CHCHCO)  deltaHrxn(T=298K) = -8.619036996920599
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8535000e+00 -1.0052000e-01 -6.4085000e-02 /
CHEB / 9.8927000e+00 8.8627000e-02 5.5913000e-02 /
CHEB / 3.4672000e-01 2.4857000e-02 1.5600000e-02 /
CHEB / 1.0127000e-01 -1.2300000e-02 -7.1033000e-03 /
CHEB / 2.4717000e-02 -7.8161000e-03 -4.8708000e-03 /

pC3H5+CO(+m)=CH2CHCHCHO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #803 (CH3CHCHCO)  deltaHrxn(T=298K) = -29.416850504671082
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.0101000e+00 -8.8638000e-01 -1.4746000e-01 /
CHEB / 4.0674000e+00 8.8169000e-01 7.1141000e-02 /
CHEB / 4.1771000e-01 1.0252000e-01 8.3269000e-02 /
CHEB / 6.6835000e-02 -6.4304000e-02 6.1008000e-03 /
CHEB / 2.3183000e-02 -5.0767000e-02 -1.5201000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H5O3J(1)  -22.68      94.52 27.47 33.26 37.77 41.38 46.86 50.82
      56.49 null
!     C4H5O3J(2)  -12.01      96.11 29.18 34.89 39.38 42.95 48.24 51.88
      56.81 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
```

```
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     CH3CHCHCO   14.06 75.12 22.13 26.48 30.11 33.1  37.72 41.11 46.34
!MRH CBS-QB3 w/1DHR corrections
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     pC3H4             46.16 58.99 14.37 17.14 19.55 21.6  24.93 27.49
      31.65
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H5O2J(12) -35.59      82.65 23.27 28.49 32.84 36.34 41.81 45.75
      49.89 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     CH3CHCHCO+O2=C4H5O3J(1) 1.4157154e+13      -0.15000
2.9166667e+02
!     C4H5O3J(1)=C4H5O3J(2)   2.0320555e+08      1.13906
3.4790987e+04
!     pC3H4+OCOOH=C4H5O3J(2)  5.2000000e+11      0.00000
6.5600000e+03
!     C4H5O2J(12)+O=C4H5O3J(1)      1.0000000e+13      0.00000
0.0000000e+00

C4H5O3J(2)(+m)=C4H5O3J(1)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -10.66865917734278
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1151000e+00 1.8497000e+00 -4.1382000e-01 /
CHEB / 1.8041000e-01 2.1992000e+00 -2.3569000e-01 /
CHEB / -5.1590000e+00 3.8660000e-01 1.3504000e-01 /
CHEB / -2.6618000e+00 -5.1813000e-01 1.1861000e-01 /
CHEB / -9.4607000e-01 -5.3070000e-01 -1.3686000e-02 /

CH3CHCHCO+O2(+m)=C4H5O3J(1)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/OneDe     O2_birad      deltaHrxn(T=298K) = -
37.415953310681125 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5044000e+00 2.1979000e+00 -4.7012000e-01 /
CHEB / -7.0341000e+00 2.5576000e+00 -1.7824000e-01 /
CHEB / -3.9578000e+00 6.2616000e-01 1.9662000e-01 /
CHEB / -1.9176000e+00 -2.8817000e-01 1.4587000e-01 /
CHEB / -6.8411000e-01 -3.5242000e-01 8.8581000e-03 /

CH3CHCHCO+O2(+m)=C4H5O3J(2)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -26.747294133338347
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 7.3484000e+00 -8.7979000e-02 -2.7888000e-01 /
CHEB / -2.5149000e+00 2.3495000e+00 -7.7280000e-02 /
CHEB / -3.0090000e+00 7.8956000e-01 1.0793000e-01 /
CHEB / -1.9260000e+00 2.7556000e-03 7.0233000e-02 /
CHEB / -8.8020000e-01 -1.9408000e-01 1.3973000e-02 /

pC3H4+OCOOH(+m)=C4H5O3J(1)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -44.10508058540228
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.3604000e+00 2.0276000e+00 -8.5444000e-01 /
CHEB / -4.4123000e+00 3.7735000e+00 -1.6605000e-01 /
CHEB / -4.3645000e+00 1.0703000e+00 1.9325000e-01 /
CHEB / -2.3115000e+00 -1.1504000e-01 1.4424000e-01 /
CHEB / -9.0026000e-01 -3.2021000e-01 3.8277000e-02 /

pC3H4+OCOOH(+m)=C4H5O3J(2)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ct/H_Ct/Nd     CO_rad/NonDe      deltaHrxn(T=298K)
= -33.4364214080595 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8933000e+00 1.3546000e+00 -2.5222000e-01 /
CHEB / -3.7581000e+00 1.9831000e+00 -2.5056000e-01 /
CHEB / -3.6414000e+00 8.2288000e-01 2.6258000e-02 /
CHEB / -2.0288000e+00 7.9075000e-02 9.6272000e-02 /
CHEB / -8.9358000e-01 -1.4992000e-01 4.7937000e-02 /

CH3CHCHCO+O2(+m)=pC3H4+OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = 6.689127274721152
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7069000e+00 -1.6426000e+00 -2.8022000e-01 /
CHEB / 4.6705000e+00 1.7234000e+00 1.9163000e-01 /
CHEB / -4.5337000e-01 2.1673000e-01 1.4207000e-01 /
CHEB / -3.1486000e-01 -1.8433000e-01 1.1940000e-02 /
CHEB / -1.0706000e-01 -1.2662000e-01 -3.9139000e-02 /

C4H5O2J(12)+O(+m)=C4H5O3J(1)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/OneDe     Oa       deltaHrxn(T=298K) = -
46.72511073989314 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9262000e+00 3.6006000e+00 -8.4489000e-01 /
CHEB / -7.3981000e+00 2.8864000e+00 1.2760000e-01 /
CHEB / -4.2179000e+00 5.1757000e-01 3.4330000e-01 /
CHEB / -1.9858000e+00 -3.7614000e-01 1.5535000e-01 /
CHEB / -7.0044000e-01 -3.6380000e-01 -4.4262000e-03 /

C4H5O2J(12)+O(+m)=C4H5O3J(2)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -36.05645156255036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 7.4124000e+00 5.6236000e-01 -4.1663000e-01 /
CHEB / -3.6756000e+00 2.6701000e+00 -7.5472000e-02 /
CHEB / -3.2993000e+00 8.8174000e-01 8.5193000e-02 /
CHEB / -2.0065000e+00 2.9726000e-02 7.6357000e-02 /
CHEB / -8.8476000e-01 -1.7301000e-01 2.3326000e-02 /

C4H5O2J(12)+O(+m)=CH3CHCHCO+O2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -9.309157429212009
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2326000e+01 -6.6684000e-01 -1.9477000e-01 /
CHEB / 3.5095000e-01 7.6330000e-01 1.7249000e-01 /
CHEB / -4.2803000e-02 1.2392000e-02 7.2358000e-02 /
CHEB / -8.8533000e-02 -8.9663000e-02 -2.4627000e-02 /
CHEB / -2.4362000e-02 -3.6440000e-02 -3.0376000e-02 /

C4H5O2J(12)+O(+m)=pC3H4+OCOOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(1))   deltaHrxn(T=298K) = -2.6200301544908555
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3486000e+00 -1.4774000e+00 -2.8061000e-01 /
CHEB / 2.9015000e+00 1.6205000e+00 2.1806000e-01 /
CHEB / -1.7885000e-01 1.1457000e-01 1.2410000e-01 /
CHEB / -1.9264000e-01 -1.8972000e-01 -9.3831000e-03 /
CHEB / -5.3577000e-02 -9.4814000e-02 -4.0720000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6O3(21)  -68.91      94.3  29.52 36.1  41.32 45.47 51.58 55.79
      61.57 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H5O3J(2)  -12.01      96.11 29.18 34.89 39.38 42.95 48.24 51.88
      56.81 null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     CH3CHCHCO   2.71  74.59 22.07 26.58 30.19 33.2  37.95 41.34 45.58
      null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H5O2J(12) -35.59      82.65 23.27 28.49 32.84 36.34 41.81 45.75
      49.89 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H5O3J(1)  -22.68      94.52 27.47 33.26 37.77 41.38 46.86 50.82
      56.49 null
```

```
!Here are the path reactions and their high-P limit kinetics:
!     C4H5O3J(2)+H=C4H6O3(21) 1.4157154e+13      -0.15000
2.9166667e+02
!     pC3H5+OCOOH=C4H6O3(21)  1.4157154e+13      -0.15000
2.9166667e+02
!     CH3CHCHCO+HO2=C4H6O3(21)      1.4157154e+13      -0.15000
2.9166667e+02
!     C4H5O2J(12)+OH=C4H6O3(21)     2.0000000e+13      0.00000
0.0000000e+00
!     C4H5O3J(1)+H=C4H6O3(21) 1.4157154e+13      -0.15000
2.9166667e+02

C4H5O3J(2)+H(+m)=C4H6O3(21)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21)) High-P Limit: R_Recombination estimate:
(Average:) Cd_rad/NonDe     H_rad         deltaHrxn(T=298K) = -
105.88862324808781 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.9342000e+00 8.9346000e+00 9.1438000e-01 /
CHEB / -3.3744000e+00 9.1578000e-01 -6.2668000e-02 /
CHEB / -2.6224000e+00 7.4390000e-02 -5.3706000e-02 /
CHEB / -1.3526000e+00 -9.0621000e-02 -3.3771000e-02 /
CHEB / -6.7346000e-01 -1.1669000e-01 -2.9262000e-02 /

pC3H5+OCOOH(+m)=C4H6O3(21)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21)) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     CO_rad/NonDe          deltaHrxn(T=298K) = -
107.9188141664718 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.6530000e+00 8.9346000e+00 9.1438000e-01 /
CHEB / -3.6303000e+00 9.1578000e-01 -6.2668000e-02 /
CHEB / -2.6321000e+00 7.4390000e-02 -5.3706000e-02 /
CHEB / -1.3716000e+00 -9.0621000e-02 -3.3771000e-02 /
CHEB / -6.8600000e-01 -1.1669000e-01 -2.9262000e-02 /

C4H5O3J(2)+H(+m)=pC3H5+OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) =
2.030190918384001 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5512000e+00 -2.0016000e-03 -1.3909000e-03 /
CHEB / 4.8475000e+00 2.1827000e-03 1.5164000e-03 /
CHEB / 1.1574000e+00 1.2995000e-04 9.0755000e-05 /
CHEB / 3.2368000e-01 -2.8504000e-04 -1.9791000e-04 /
CHEB / 7.4565000e-02 -6.7401000e-05 -4.6991000e-05 /

CH3CHCHCO+HO2(+m)=C4H6O3(21)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21)) High-P Limit: R_Recombination estimate:
(Average:) CO_rad/OneDe     O_rad/NonDe         deltaHrxn(T=298K) = -
72.04253182620411 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7138000e+00 5.0866000e+00 -5.8112000e-01 /
CHEB / -4.3795000e+00 4.6361000e-01 1.7531000e-01 /
CHEB / -2.7202000e+00 1.7354000e-01 1.1720000e-01 /
CHEB / -1.4494000e+00 -9.1451000e-02 1.3562000e-02 /
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CHEB / -7.3648000e-01 -1.3059000e-01 -1.0148000e-02 /

C4H5O3J(2)+H(+m)=CH3CHCHCO+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
33.84609142188369 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2706000e+00 -1.4926000e-03 -1.0396000e-03 /
CHEB / 1.0768000e+00 1.3238000e-03 9.2216000e-04 /
CHEB / 4.4633000e-01 4.6580000e-04 3.2443000e-04 /
CHEB / 1.9719000e-01 -1.7037000e-04 -1.1877000e-04 /
CHEB / 6.5484000e-02 -1.4011000e-04 -9.7599000e-05 /

pC3H5+OCOOH(+m)=CH3CHCHCO+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
35.87628234026769 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5518000e+00 -1.4926000e-03 -1.0396000e-03 /
CHEB / 8.2088000e-01 1.3238000e-03 9.2216000e-04 /
CHEB / 4.3660000e-01 4.6580000e-04 3.2443000e-04 /
CHEB / 1.7824000e-01 -1.7037000e-04 -1.1877000e-04 /
CHEB / 5.2942000e-02 -1.4011000e-04 -9.7599000e-05 /

C4H5O2J(12)+OH(+m)=C4H6O3(21)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/OneDe     O_pri_rad      deltaHrxn(T=298K) = -
42.63548877778435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1671000e+01 6.6446000e-01 -4.1498000e-02 /
CHEB / -3.2339000e+00 1.0329000e+00 -2.2280000e-02 /
CHEB / -2.3000000e+00 4.7288000e-01 4.7315000e-02 /
CHEB / -1.4041000e+00 6.1972000e-02 4.4475000e-02 /
CHEB / -7.5183000e-01 -1.0073000e-01 6.1359000e-03 /

C4H5O3J(2)+H(+m)=C4H5O2J(12)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
63.25313447030344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2721000e+01 4.1794000e-07 2.8823000e-07 /
CHEB / -3.1301000e-03 4.3406000e-07 3.0279000e-07 /
CHEB / -4.1663000e-03 2.5899000e-07 1.8362000e-07 /
CHEB / 4.9179000e-02 1.7877000e-07 1.2444000e-07 /
CHEB / 2.7871000e-02 1.3653000e-07 9.3518000e-08 /

pC3H5+OCOOH(+m)=C4H5O2J(12)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
65.28332538868744 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3002000e+01 4.1794000e-07 2.8823000e-07 /
CHEB / -2.5901000e-01 4.3406000e-07 3.0279000e-07 /
CHEB / -1.3888000e-02 2.5899000e-07 1.8362000e-07 /
CHEB / 3.0222000e-02 1.7877000e-07 1.2444000e-07 /
CHEB / 1.5329000e-02 1.3653000e-07 9.3518000e-08 /
```

```
CH3CHCHCO+HO2(+m)=C4H5O2J(12)+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1243 (C4H6O3(21)) deltaHrxn(T=298K) = -
29.40704304841976 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3024000e+01 -9.3910000e-02 -6.6569000e-02 /
CHEB / -2.8365000e-01 1.0992000e-01 7.7097000e-02 /
CHEB / -2.0737000e-02 2.1996000e-03 2.3608000e-03 /
CHEB / -2.8390000e-03 -1.8730000e-02 -1.2546000e-02 /
CHEB / -1.5447000e-03 -3.4722000e-03 -3.1609000e-03 /

C4H5O3J(1)+H(+m)=C4H6O3(21)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
95.21996407074502 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9497000e-01 8.2607000e+00 5.4201000e-01 /
CHEB / -4.2240000e+00 5.7077000e-01 -1.8160000e-01 /
CHEB / -2.6930000e+00 2.0889000e-02 -3.7114000e-02 /
CHEB / -1.3873000e+00 -1.0513000e-01 -2.2025000e-02 /
CHEB / -6.9455000e-01 -1.2549000e-01 -2.5549000e-02 /

C4H5O3J(2)+H(+m)=C4H5O3J(1)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
10.668659177342782 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3788000e+00 -2.3692000e-03 -1.6466000e-03 /
CHEB / 1.8590000e+00 2.4929000e-03 1.7321000e-03 /
CHEB / 6.6373000e-01 2.9515000e-04 2.0545000e-04 /
CHEB / 1.9368000e-01 -3.5495000e-04 -2.4643000e-04 /
CHEB / 3.2000000e-02 -1.2448000e-04 -8.6627000e-05 /

C4H5O3J(1)+H(+m)=pC3H5+OCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) =
12.698850095726776 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9607000e+00 -2.3692000e-03 -1.6466000e-03 /
CHEB / 6.5884000e+00 2.4929000e-03 1.7321000e-03 /
CHEB / 9.7342000e-01 2.9515000e-04 2.0545000e-04 /
CHEB / 2.9001000e-01 -3.5495000e-04 -2.4643000e-04 /
CHEB / 6.4088000e-02 -1.2448000e-04 -8.6627000e-05 /

C4H5O3J(1)+H(+m)=CH3CHCHCO+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
23.17743224454091 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4462000e+00 -5.5258000e-03 -3.8478000e-03 /
CHEB / 8.4808000e-01 5.7239000e-03 3.9862000e-03 /
CHEB / 5.2607000e-01 9.2222000e-04 6.4150000e-04 /
CHEB / 1.9322000e-01 -9.2028000e-04 -6.4074000e-04 /
CHEB / 5.2523000e-02 -3.5563000e-04 -2.4754000e-04 /
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C4H5O3J(1)+H(+m)=C4H5O2J(12)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1243 (C4H6O3(21))      deltaHrxn(T=298K) = -
52.58447529296067 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3411000e+01 -2.7746000e-05 -2.3645000e-05 /
CHEB / -5.8553000e-01 2.0746000e-05 1.7585000e-05 /
CHEB / -1.0424000e-02 2.1904000e-05 1.8594000e-05 /
CHEB / 3.7203000e-02 -1.0294000e-05 -8.7718000e-06 /
CHEB / 1.9011000e-02 -7.7089000e-06 -6.5693000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H5O2J(12) -35.59      82.65 23.27 28.49 32.84 36.34 41.81 45.75
      49.89 null
!     pC3H5             63.75 65.2  15.26 18.48 21.36 23.87 27.92 31.0
      35.86 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3CHCHCO   2.71  74.59 22.07 26.58 30.19 33.2  37.95 41.34 45.58
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     pC3H5+CO2=C4H5O2J(12)   3.2847733e+07      1.50370
7.3354000e+03
!     CH3CHCHCO+O=C4H5O2J(12) 1.0000000e+13      0.00000
0.0000000e+00

C4H5O2J(12)(+m)=pC3H5+CO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1443 (C4H5O2J(12))     deltaHrxn(T=298K) =
5.289364355550333 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.5808000e+00 1.7634000e+00 -1.2483000e-01 /
CHEB / 8.9303000e-03 2.0866000e-01 1.1313000e-01 /
CHEB / -2.0888000e+00 1.5082000e-02 7.9351000e-03 /
CHEB / -9.1023000e-01 -1.1467000e-02 -7.6273000e-03 /
CHEB / -3.9734000e-01 -3.5935000e-03 -2.1890000e-03 /

CH3CHCHCO+O(+m)=C4H5O2J(12)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1443 (C4H5O2J(12)) High-P Limit: Oa_R_Recombination
estimate: (Average:) CO_rad/OneDe     Oa        deltaHrxn(T=298K) = -
97.8395957739758 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0630000e+01 3.1051000e+00 5.3440000e-01 /
CHEB / -4.7566000e+00 -4.9399000e-01 -2.1416000e-01 /
CHEB / -2.0235000e+00 -1.1636000e-01 -5.7982000e-02 /
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CHEB / -8.4561000e-01 -2.3088000e-02 -1.2573000e-02 /
CHEB / -3.7404000e-01 -2.0998000e-03 -1.1829000e-03 /

CH3CHCHCO+O(+m)=pC3H5+CO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1443 (C4H5O2J(12))     deltaHrxn(T=298K) = -
92.55023141842548 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3680000e+01 1.4221000e-09 9.8989000e-10 /
CHEB / -5.3871000e-01 6.5919000e-10 4.5884000e-10 /
CHEB / 2.1471000e-03 6.0798000e-10 4.2319000e-10 /
CHEB / 2.1108000e-02 6.2876000e-10 4.3767000e-10 /
CHEB / 9.0942000e-03 5.3502000e-10 3.7241000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6O3(3)   -41.95      95.75 29.87 36.11 41.36 45.35 51.63 56.13
      60.26 null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C2H3             71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H5O2J(54) 21.86 78.59 23.19 28.36 32.19 35.33 39.81 42.82 47.49
      null
!     HCO              10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!     HO2              0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     C4H5O2J(13) -6.19 86.99 24.08 29.28 33.8  37.19 42.8  46.53 49.88
      null
!     OH               9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H5O3J(3)  -5.85 95.97 27.82 33.27 37.81 41.26 46.91 51.16 55.18
      null
!     CO               -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     C3H5O2J(54)+HCO=C4H6O3(3)     1.4157154e+13      -0.15000
2.9166667e+02
!     CH2CHCHCHO+HO2=C4H6O3(3)      1.4157154e+13      -0.15000
2.9166667e+02
!     C4H5O2J(13)+OH=C4H6O3(3)      2.0000000e+13      0.00000
0.0000000e+00
!     C4H5O3J(3)+H=C4H6O3(3)  1.4157154e+13      -0.15000
2.9166667e+02

C3H5O2J(54)+HCO(+m)=C4H6O3(3)(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeO     CO_pri_rad        deltaHrxn(T=298K) = -
74.20229912377937 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.0062000e+01 1.9709000e+00 -1.9784000e-02 /
CHEB / -1.6097000e+00 2.8317000e-02 1.9206000e-02 /
CHEB / -5.1563000e-01 6.6945000e-03 4.5246000e-03 /
CHEB / -5.4597000e-02 -5.3986000e-03 -3.6042000e-03 /
CHEB / 5.3998000e-02 -2.4571000e-03 -1.6612000e-03 /

CH2CHCHCHO+HO2(+m)=C4H6O3(3)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/TwoDe     O_rad/NonDe        deltaHrxn(T=298K) = -
50.28495103478623 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1254000e+01 1.2075000e+00 -1.9891000e-01 /
CHEB / -1.9241000e+00 7.2271000e-01 1.4771000e-01 /
CHEB / -8.9576000e-01 1.7879000e-01 6.0009000e-02 /
CHEB / -2.7060000e-01 -6.0003000e-02 7.7664000e-03 /
CHEB / -3.4951000e-02 -5.3980000e-02 -1.1098000e-02 /

C3H5O2J(54)+HCO(+m)=CH2CHCHCHO+HO2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1626 (C4H6O3(3))  deltaHrxn(T=298K) = -
23.91734808899314 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1075000e+01 -2.3869000e-02 -1.6240000e-02 /
CHEB / -6.7002000e-02 2.7088000e-02 1.8398000e-02 /
CHEB / 1.4412000e-01 1.4619000e-03 1.0098000e-03 /
CHEB / 6.3886000e-02 -5.2500000e-03 -3.5290000e-03 /
CHEB / 2.6939000e-02 -6.8775000e-04 -4.8897000e-04 /

C4H5O2J(13)+OH(+m)=C4H6O3(3)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     O_pri_rad      deltaHrxn(T=298K) = -
45.07524014769287 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3111000e+01 7.1005000e-01 -6.4323000e-02 /
CHEB / -2.4637000e+00 9.8416000e-01 -2.0090000e-02 /
CHEB / -9.8248000e-01 3.6633000e-01 4.7310000e-02 /
CHEB / -3.6792000e-01 2.2923000e-02 3.4972000e-02 /
CHEB / -7.8223000e-02 -5.3869000e-02 4.2023000e-03 /

C3H5O2J(54)+HCO(+m)=C4H5O2J(13)+OH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1626 (C4H6O3(3))  deltaHrxn(T=298K) = -
29.12705897608651 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3243000e+01 -2.5153000e-02 -1.7105000e-02 /
CHEB / -4.5926000e-01 2.7684000e-02 1.8796000e-02 /
CHEB / -7.1553000e-03 2.6767000e-03 1.8268000e-03 /
CHEB / 2.1181000e-02 -5.5274000e-03 -3.7095000e-03 /
CHEB / 1.4527000e-02 -1.1083000e-03 -7.6946000e-04 /

CH2CHCHCHO+HO2(+m)=C4H5O2J(13)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1626 (C4H6O3(3))  deltaHrxn(T=298K) = -
5.2097108870933635 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 1.2397000e+01 -5.7514000e-01 -1.6815000e-01 /
CHEB / 3.4938000e-01 6.7655000e-01 1.6891000e-01 /
CHEB / -5.9792000e-02 -1.2329000e-02 3.3028000e-02 /
CHEB / -8.0065000e-02 -8.7842000e-02 -2.1287000e-02 /
CHEB / -1.8019000e-02 -1.8347000e-02 -1.7977000e-02 /

C4H5O3J(3)+H(+m)=C4H6O3(3)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) High-P Limit: R_Recombination estimate:
(Average:) O_rad/NonDe     H_rad          deltaHrxn(T=298K) = -
85.09098369335389 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0965000e+00 1.9956000e+00 -3.0726000e-03 /
CHEB / -1.0451000e+00 3.9492000e-03 2.7390000e-03 /
CHEB / -3.8182000e-01 1.1755000e-03 8.1505000e-04 /
CHEB / 1.0033000e-02 -7.4179000e-04 -5.1322000e-04 /
CHEB / 7.8756000e-02 -4.1712000e-04 -2.8919000e-04 /

C4H5O3J(3)+H(+m)=C3H5O2J(54)+HCO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1626 (C4H6O3(3))  deltaHrxn(T=298K) = -
10.888684569574522 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2669000e+00 -3.2512000e-03 -2.2566000e-03 /
CHEB / 1.6603000e+00 3.6272000e-03 2.5167000e-03 /
CHEB / 6.3423000e-01 1.5288000e-04 1.0683000e-04 /
CHEB / 2.1343000e-01 -6.3221000e-04 -4.3820000e-04 /
CHEB / 7.4952000e-02 -1.0209000e-04 -7.1386000e-05 /

C4H5O3J(3)+H(+m)=CH2CHCHCHO+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) deltaHrxn(T=298K) = -34.806032658567666
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0972000e+01 -3.9089000e-03 -2.7124000e-03 /
CHEB / 6.6793000e-02 3.9577000e-03 2.7453000e-03 /
CHEB / 1.1542000e-01 7.0237000e-04 4.8748000e-04 /
CHEB / 8.4551000e-02 -7.8539000e-04 -5.4380000e-04 /
CHEB / 3.9177000e-02 -2.6686000e-04 -1.8543000e-04 /

C4H5O3J(3)+H(+m)=C4H5O2J(13)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1626 (C4H6O3(3)) deltaHrxn(T=298K) = -40.01574354566103
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2952000e+01 -4.0185000e-03 -2.7883000e-03 /
CHEB / -1.9922000e-01 3.9781000e-03 2.7594000e-03 /
CHEB / -1.4767000e-03 8.0894000e-04 5.6128000e-04 /
CHEB / 4.5034000e-02 -7.8765000e-04 -5.4528000e-04 /
CHEB / 2.6090000e-02 -3.0194000e-04 -2.0968000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
```

```
!Here are the species and their thermochemistry:
!     C4H5O2J(13) -6.19 86.99 24.08 29.28 33.8  37.19 42.8  46.53 49.88
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2CHCH2O   22.15 72.99 17.7  21.45 24.85 27.83 32.58 36.01 41.06
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+HCO=C4H5O2J(13)   5.2000000e+11      0.00000
6.5600000e+03
!     CH2CHCH2O+CO=C4H5O2J(13)      5.9198482e+04      2.36750
7.2970000e+04
!     CH2CHCHCHO+O=C4H5O2J(13)      1.0000000e+13      0.00000
0.0000000e+00

C4H5O2J(13)(+m)=C3H4O+HCO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13))     deltaHrxn(T=298K) = -
3.729860552418451 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7307000e+00 1.9999000e+00 -3.9493000e-05 /
CHEB / 1.0412000e-01 -3.6593000e-05 -2.5457000e-05 /
CHEB / -2.0194000e+00 -1.1175000e-05 -7.7683000e-06 /
CHEB / -8.7129000e-01 -4.2158000e-06 -2.9279000e-06 /
CHEB / -3.7778000e-01 -2.1330000e-06 -1.4807000e-06 /

C4H5O2J(13)(+m)=CH2CHCH2O+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13))     deltaHrxn(T=298K) =
1.9196623357604814 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.6102000e+01 2.0059000e+00 4.1282000e-03 /
CHEB / 2.2906000e+01 5.8482000e-03 4.0687000e-03 /
CHEB / -1.6520000e+00 2.9089000e-03 2.0234000e-03 /
CHEB / -7.4500000e-01 1.4774000e-03 1.0274000e-03 /
CHEB / -3.3448000e-01 7.6052000e-04 5.2878000e-04 /

CH2CHCH2O+CO(+m)=C3H4O+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13))     deltaHrxn(T=298K) = -
5.649522888178932 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8675000e+01 2.0717000e-08 1.4420000e-08 /
CHEB / 2.5890000e+01 3.7499000e-08 2.6102000e-08 /
CHEB / 2.6177000e-01 2.9201000e-08 2.0326000e-08 /
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CHEB / 9.5049000e-02 2.0144000e-08 1.4022000e-08 /
CHEB / 2.9094000e-02 1.2471000e-08 8.6811000e-09 /

CH2CHCHCHO+O(+m)=C4H5O2J(13)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13)) High-P Limit: Oa_R_Recombination
estimate: (Average:) C_rad/H/TwoDe     Oa       deltaHrxn(T=298K) = -
73.64226361264942 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3438000e+01 2.0056000e+00 3.9026000e-03 /
CHEB / -3.7927000e+00 5.5282000e-03 3.8460000e-03 /
CHEB / -1.6865000e+00 2.7496000e-03 1.9125000e-03 /
CHEB / -7.5014000e-01 1.3964000e-03 9.7105000e-04 /
CHEB / -3.3820000e-01 7.1871000e-04 4.9970000e-04 /

CH2CHCHCHO+O(+m)=C3H4O+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13))     deltaHrxn(T=298K) = -
77.37212416506786 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3961000e+01 1.8738000e-08 1.3043000e-08 /
CHEB / -8.2040000e-01 3.4200000e-08 2.3806000e-08 /
CHEB / -2.3481000e-02 2.7062000e-08 1.8837000e-08 /
CHEB / -1.0995000e-02 1.9059000e-08 1.3266000e-08 /
CHEB / -1.2484000e-02 1.2103000e-08 8.4248000e-09 /

CH2CHCHCHO+O(+m)=CH2CHCH2O+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1855 (C4H5O2J(13))     deltaHrxn(T=298K) = -
71.72260127688892 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2711000e+00 -5.7936000e-06 -4.0328000e-06 /
CHEB / 4.9546000e+00 3.2163000e-06 2.2388000e-06 /
CHEB / 1.2118000e+00 1.8334000e-06 1.2762000e-06 /
CHEB / 3.4507000e-01 3.2508000e-07 2.2628000e-07 /
CHEB / 1.0418000e-01 -4.5649000e-08 -3.1774000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7O3J(1)  -48.72      94.45 30.68 37.09 42.16 46.31 53.03 57.8
      65.1  null
!     C4H7O3J(2)  -48.6 99.36 31.19 37.16 42.22 46.5  53.4  58.13 65.54
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
!     C4H7OJ(8)         -12.53      83.27 24.09 28.93 33.21 36.9  43.23
      47.78 53.46 null
```

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!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     C4H6O3(21)  -68.91      94.3  29.52 36.1  41.32 45.47 51.58 55.79
      61.57 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     C4H7OJ(8)+O2=C4H7O3J(1) 1.5050000e+12      0.00000
0.0000000e+00
!     C4H7O3J(1)=C4H7O3J(2)   5.0000000e+10      0.00000
2.0850000e+04
!     C3H6+OCOOH=C4H7O3J(2)   5.2000000e+11      0.00000
6.5600000e+03
!     C4H6O3(21)+H=C4H7O3J(2) 2.8500000e+13      0.00000
4.3000000e+03

C4H7O3J(1)(+m)=C4H7O3J(2)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1)) High-P Limit: intra_H_migration estimate:
(Average:) R5H_SSSS     O_rad_out     Cs_H_out_H/NonDeC
      deltaHrxn(T=298K) = 0.11988629071475998 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3696000e+00 4.9065000e-01 -2.6073000e-02 /
CHEB / -1.2176000e+00 6.7831000e-01 -2.2380000e-02 /
CHEB / -5.5392000e+00 3.8415000e-02 2.2130000e-02 /
CHEB / -3.0826000e+00 -4.2307000e-01 2.3669000e-02 /
CHEB / -1.1300000e+00 -4.2789000e-01 -9.4583000e-03 /

C4H7OJ(8)+O2(+m)=C4H7O3J(1)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1)) High-P Limit: R_Recombination exact:
CO_rad/NonDe     O2_birad           deltaHrxn(T=298K) = -
36.86611699057335 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3414000e+00 1.2548000e+00 -1.8476000e-01 /
CHEB / -7.0770000e+00 1.6369000e+00 -9.8927000e-02 /
CHEB / -4.2727000e+00 4.7113000e-01 5.5612000e-02 /
CHEB / -2.2313000e+00 -1.8024000e-01 3.2712000e-02 /
CHEB / -8.2909000e-01 -2.6013000e-01 -1.9275000e-02 /

C4H7OJ(8)+O2(+m)=C4H7O3J(2)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -36.74623069985859
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.4868000e+00 -2.6926000e-01 -2.0103000e-01 /
CHEB / -5.4591000e+00 2.1483000e+00 -2.4122000e-02 /
CHEB / -3.9620000e+00 5.6695000e-01 1.2591000e-01 /
CHEB / -2.3836000e+00 -2.1512000e-01 5.6350000e-02 /
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CHEB / -1.0354000e+00 -2.9985000e-01 -1.5030000e-02 /

C3H6+OCOOH(+m)=C4H7O3J(1)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -30.226824897219036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.4601000e+00 -3.7956000e-01 -1.8428000e-01 /
CHEB / -3.9554000e+00 1.9758000e+00 -7.6151000e-03 /
CHEB / -4.2120000e+00 4.7226000e-01 1.1919000e-01 /
CHEB / -2.3356000e+00 -2.5470000e-01 4.3018000e-02 /
CHEB / -9.0940000e-01 -2.9854000e-01 -2.6259000e-02 /

C3H6+OCOOH(+m)=C4H7O3J(2)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/Nd     CO_rad/NonDe
      deltaHrxn(T=298K) = -30.106938606504276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7927000e+00 8.6356000e-01 -8.2524000e-02 /
CHEB / -3.6632000e+00 1.1543000e+00 -9.7923000e-03 /
CHEB / -3.6936000e+00 3.8275000e-01 6.0915000e-02 /
CHEB / -2.0634000e+00 -7.9343000e-02 3.8728000e-02 /
CHEB / -8.5953000e-01 -1.7103000e-01 -2.8148000e-03 /

C4H7OJ(8)+O2(+m)=C3H6+OCOOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -6.639292093354317
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0164000e+01 -1.7850000e+00 -2.3577000e-01 /
CHEB / 5.0211000e-01 1.9730000e+00 1.4830000e-01 /
CHEB / -6.5675000e-01 1.6604000e-01 1.5134000e-01 /
CHEB / -3.9325000e-01 -2.6166000e-01 -4.3184000e-03 /
CHEB / -1.0689000e-01 -1.6362000e-01 -4.5542000e-02 /

C4H6O3(21)+H(+m)=C4H7O3J(1)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -31.906238705024663
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2615000e+00 -5.4772000e-01 -1.4229000e-01 /
CHEB / -4.4854000e+00 1.8863000e+00 -1.8924000e-02 /
CHEB / -4.1456000e+00 4.8661000e-01 1.0974000e-01 /
CHEB / -2.3498000e+00 -2.4686000e-01 4.7093000e-02 /
CHEB / -9.1994000e-01 -3.0408000e-01 -2.3451000e-02 /

C4H6O3(21)+H(+m)=C4H7O3J(2)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H/De_Cd/H/Nd     H_rad        deltaHrxn(T=298K)
= -31.786352414309903 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7216000e+00 7.3204000e-01 -5.3189000e-02 /
CHEB / -4.3268000e+00 1.0455000e+00 -9.4115000e-03 /
CHEB / -3.6202000e+00 3.7907000e-01 5.1379000e-02 /
CHEB / -2.0585000e+00 -6.3982000e-02 3.8316000e-02 /
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CHEB / -8.6306000e-01 -1.6709000e-01 2.0405000e-04 /

C4H7OJ(8)+O2(+m)=C4H6O3(21)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -4.95987828554869
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1120000e+00 -1.8677000e+00 -2.2108000e-01 /
CHEB / 1.1931000e+00 2.0320000e+00 1.2249000e-01 /
CHEB / -4.5079000e-01 2.1481000e-01 1.5517000e-01 /
CHEB / -3.4134000e-01 -2.6758000e-01 6.5477000e-03 /
CHEB / -8.5742000e-02 -1.8250000e-01 -4.2133000e-02 /

C4H6O3(21)+H(+m)=C3H6+OCOOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(1))   deltaHrxn(T=298K) = -1.679413807805627
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1112000e+01 -9.6012000e-01 -1.0918000e-01 /
CHEB / 2.3729000e+00 1.0453000e+00 5.3458000e-02 /
CHEB / -2.5702000e-01 1.0765000e-01 8.8862000e-02 /
CHEB / -1.7928000e-01 -1.4328000e-01 2.3766000e-03 /
CHEB / -3.3277000e-02 -8.4913000e-02 -2.9010000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7O3J(3)        -29.08      96.99 30.93 37.84 43.34 47.45 53.78
      58.63 65.27 Estimated by Group Additivity
!     C4H7O3J(4)        -33.6 95.73 31.97 38.51 44.06 48.31 54.94 59.87
      66.09 Estimated by Group Additivity
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21 Primary Thermo Library: CFG (Species ID: CH3)
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96  Primary Thermo Library: CFG (Species ID: H)
!     C2H3O-1           32.17 62.75 14.65 17.72 20.0  21.59 23.58 24.88
      27.02 Primary Thermo Library: CFG (Species ID: CHCHOH)
!     C4H7O_1_2         -8.74 77.49 22.98 28.87 33.91 38.04 44.26 48.73
      55.61 Estimated by Group Additivity
!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
      Primary Thermo Library: CFG (Species ID: O2)
!     OH          8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23  7.72
      Primary Thermo Library: CFG (Species ID: OH)
!     CH3CHCHCHO        -28.19      75.98 22.26 27.43 31.78 35.41 41.16
      45.23 50.19 Estimated by Group Additivity
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25 Primary Thermo Library: CFG (Species ID: HO2)
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
      Primary Thermo Library: CFG (Species ID: O)
!     CH2CHCHCHOH       -16.05      75.67 23.07 28.9  33.47 36.92 41.89
      45.42 51.05 Estimated by Group Additivity
!Here are the path reactions and their high-P limit kinetics:
!     C4H7O_1_2+O2=C4H7O3J(3) 3.770e+12     0.00        0.00
!     C4H7O3J(3)=C4H7O3J(4)         2.032e+08     1.14        34790.99
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!     CH3CHCHCHO+HO2=C4H7O3J(4)     1.000e+11     0.00        11000.00
!     C4H7O3J(3)=CH2CHCHCHOH+HO2    9.904e+06     1.83        24247.00

C4H7O3J(3)(+m)=C4H7O3J(4)(+m)                  1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3)) High-P Limit:
intra_H_migration estimate: (Average:) [ R6H_RSSMS , O_rad_out , O_H_out
]
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3655000e+01  6.7668000e+00 -1.1100000e+00 /
CHEB /  3.5845000e+00 -6.4038000e-01  3.9889000e-01 /
CHEB / -5.3061000e+00 -7.1453000e-01  1.1343000e-01 /
CHEB / -2.3490000e+00 -6.4620000e-01 -8.6676000e-02 /
CHEB / -6.5016000e-01 -2.8543000e-01 -1.1063000e-01 /
! For the above reaction, deltaHrxn(T=298K) = -4.5 kcal/mol

C4H7O_1_2+O2(+m)=C4H7O3J(3)(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3)) High-P Limit:
R_Recombination estimate: (Average:) [ C_rad/H/OneDeC , O2_birad ]
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  9.4563000e+00  9.2244000e-01 -6.8617000e-02 /
CHEB / -5.5624000e+00  1.1009000e+00  2.6643000e-02 /
CHEB / -3.4768000e+00  1.6692000e-01  7.2487000e-02 /
CHEB / -1.7228000e+00 -2.2000000e-01  5.9558000e-04 /
CHEB / -6.3737000e-01 -1.7625000e-01 -3.9733000e-02 /
! For the above reaction, deltaHrxn(T=298K) = -21.0 kcal/mol

C4H7O_1_2+O2(+m)=C4H7O3J(4)(+m)                1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1809000e+00  4.5754000e+00 -5.9548000e-01 /
CHEB /  1.9458000e-02  3.9396000e-01  4.0591000e-01 /
CHEB / -3.3630000e+00 -2.0466000e-01  1.1415000e-01 /
CHEB / -1.6082000e+00 -3.2021000e-01 -6.2753000e-02 /
CHEB / -5.4266000e-01 -1.2749000e-01 -8.4773000e-02 /
! For the above reaction, deltaHrxn(T=298K) = -25.5 kcal/mol

C4H7O3J(3)(+m)=CH3CHCHCHO+HO2(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.3501000e+00  3.1947000e+00 -5.9780000e-01 /
CHEB /  6.1281000e+00  8.9213000e-01  4.1226000e-01 /
CHEB / -3.5892000e+00 -3.1936000e-02  1.1572000e-01 /
CHEB / -1.7473000e+00 -3.0010000e-01 -3.3718000e-02 /
CHEB / -6.4957000e-01 -1.7743000e-01 -5.4950000e-02 /
! For the above reaction, deltaHrxn(T=298K) = +4.0 kcal/mol

C4H7O3J(4)(+m)=CH3CHCHCHO+HO2(+m)              1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  1.9949000e+00  1.0319000e+00 -8.4383000e-02 /
CHEB / -1.8580000e-01  1.0961000e+00  4.7227000e-02 /
CHEB / -3.9306000e+00  1.2637000e-01  6.6797000e-02 /
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CHEB / -1.7548000e+00 -2.0013000e-01 -1.2428000e-02 /
CHEB / -5.5933000e-01 -1.2403000e-01 -4.3212000e-02 /
! For the above reaction, deltaHrxn(T=298K) = +8.5 kcal/mol

C4H7O_1_2+O2(+m)=CH3CHCHCHO+HO2(+m)             1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  4.4234000e+00 -3.2266000e-01 -1.7971000e-01 /
CHEB /  5.5650000e+00  4.0711000e-01  2.1875000e-01 /
CHEB / -7.1967000e-02 -3.2304000e-02 -4.8788000e-03 /
CHEB / -2.2652000e-01 -6.1152000e-02 -3.5818000e-02 /
CHEB / -1.7640000e-01 -8.6849000e-03 -9.8950000e-03 /
! For the above reaction, deltaHrxn(T=298K) = -17.1 kcal/mol

CH2CHCHCHOH+HO2(+m)=C4H7O3J(3)(+m)        1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  3.1216000e+00  1.1576000e+00 -1.2761000e-01 /
CHEB / -1.7218000e+00  1.1777000e+00  5.6260000e-02 /
CHEB / -3.1080000e+00  1.3767000e-01  8.5589000e-02 /
CHEB / -1.5607000e+00 -2.3682000e-01 -3.2742000e-03 /
CHEB / -5.6415000e-01 -1.7752000e-01 -4.2155000e-02 /
! For the above reaction, deltaHrxn(T=298K) = -16.1 kcal/mol

CH2CHCHCHOH+HO2(+m)=C4H7O3J(4)(+m)        1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.9901000e+00  4.6521000e+00 -5.7424000e-01 /
CHEB /  3.4022000e+00  4.6155000e-01  4.0893000e-01 /
CHEB / -2.9059000e+00 -2.0121000e-01  1.1104000e-01 /
CHEB / -1.4294000e+00 -3.1985000e-01 -6.2630000e-02 /
CHEB / -4.6734000e-01 -1.2518000e-01 -8.4219000e-02 /
! For the above reaction, deltaHrxn(T=298K) = -20.6 kcal/mol

C4H7O_1_2+O2(+m)=CH2CHCHCHOH+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  9.3443000e+00 -7.0985000e-01 -1.4468000e-01 /
CHEB /  2.9829000e+00  8.7306000e-01  1.3361000e-01 /
CHEB /  1.7052000e-01 -3.8676000e-02  6.4077000e-02 /
CHEB / -5.8866000e-02 -1.3126000e-01 -3.6471000e-02 /
CHEB / -3.7443000e-02 -3.5978000e-02 -3.3483000e-02 /
! For the above reaction, deltaHrxn(T=298K) = -4.9 kcal/mol

CH2CHCHCHOH+HO2(+m)=CH3CHCHCHO+HO2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O3J(3))
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2222000e+00 -3.2118000e-01 -1.7455000e-01 /
CHEB /  9.0851000e+00  4.0575000e-01  2.1239000e-01 /
CHEB /  4.1611000e-01 -3.6231000e-02 -6.3875000e-03 /
CHEB / -4.4516000e-02 -5.7163000e-02 -3.3156000e-02 /
CHEB / -1.0100000e-01 -6.3562000e-03 -8.1804000e-03 /
```

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! For the above reaction, deltaHrxn(T=298K) = -12.1 kcal/mol

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H7O3J(5)  -22.75      99.94 30.08 36.75 42.11 46.24 52.84 57.9
      62.75 null
!     C4H7O3J(6)  -6.89 98.26 31.15 38.29 44.05 48.44 55.18 60.07 64.24
      null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     CH2OH            -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C4H7O-13         -2.41 79.66 27.06 31.99 36.04 39.42 44.8  48.92
      55.62  !MRH CBS-QB3 w/1DHR corrections
!     O2               0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H4O            -29.12      62.18 15.02 18.07 20.54 22.51 25.45
      27.61 31.14
!     H2O              -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C3H5O2J(54) 21.86 78.59 23.19 28.36 32.19 35.33 39.81 42.82 47.49
      null
!     CH2O             -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     C4H6O3(3)   -41.95      95.75 29.87 36.11 41.36 45.35 51.63 56.13
      60.26 null
!     HO2              3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2CHCHCHOH -16.05      75.67 23.07 28.9  33.47 36.92 41.89 45.42
      51.05 null
!Here are the path reactions and their high-P limit kinetics:
!     C4H7O-13+O2=C4H7O3J(5)  3.7700000e+12      0.00000
0.0000000e+00
!     C4H7O3J(6)=C4H7O3J(5)   2.0320555e+08      1.13906
3.4790987e+04
!     C3H5O2J(54)+CH2O=C4H7O3J(6)   1.0000000e+11      0.00000
1.1900000e+04
!     C4H6O3(3)+H=C4H7O3J(6)  1.0000000e+11      0.00000
1.1900000e+04
!     C4H7O3J(5)=CH2CHCHCHOH+HO2    1.6008111e+11      0.56333
2.9800000e+04

C4H7O3J(6)(+m)=C4H7O3J(5)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5)) High-P Limit: intra_H_migration estimate:
(Average:) R5H_SSSS     O_rad_out     O_H_out         deltaHrxn(T=298K)
= -15.858251776831164 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

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CHEB / 5    3 /
CHEB / -2.1101000e+01 1.1430000e+01 3.4124000e-01 /
CHEB / 5.3524000e+00 -1.0889000e+00 1.0721000e-02 /
CHEB / -3.7736000e+00 -1.0282000e+00 3.6975000e-02 /
CHEB / -1.6712000e+00 -5.6022000e-01 -3.1952000e-02 /
CHEB / -6.2156000e-01 -1.3362000e-01 -6.0674000e-02 /

C4H7O-13+O2(+m)=C4H7O3J(5)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     O2_birad          deltaHrxn(T=298K) = -
21.01733182668477 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4047000e+00 9.7061000e-01 -7.4516000e-02 /
CHEB / -5.3600000e+00 1.1088000e+00 3.7761000e-02 /
CHEB / -3.3353000e+00 1.6682000e-01 6.7419000e-02 /
CHEB / -1.6059000e+00 -1.9348000e-01 -3.6442000e-03 /
CHEB / -5.9056000e-01 -1.4345000e-01 -3.6277000e-02 /

C4H7O3J(6)(+m)=C4H7O-13+O2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = 5.159080049853608
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2693000e+01 5.0487000e+00 6.4182000e-01 /
CHEB / 8.0711000e+00 2.8762000e-02 -1.0782000e-01 /
CHEB / -2.1968000e+00 -2.3278000e-01 -4.9123000e-02 /
CHEB / -1.0264000e+00 -1.3321000e-01 -3.5089000e-02 /
CHEB / -4.8379000e-01 -2.2953000e-02 -5.0120000e-03 /

C3H5O2J(54)+CH2O(+m)=C4H7O3J(5)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -18.387994398224944
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4922000e+01 6.9875000e+00 -2.8782000e-02 /
CHEB / 5.2648000e+00 -3.1479000e-01 4.8168000e-01 /
CHEB / -3.2420000e+00 -5.7487000e-01 1.7762000e-01 /
CHEB / -1.4687000e+00 -4.3057000e-01 1.2347000e-02 /
CHEB / -5.6160000e-01 -1.3412000e-01 -4.0707000e-02 /

C4H7O3J(6)(+m)=C3H5O2J(54)+CH2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = 2.5297426213937797
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8817000e+00 1.3246000e+00 -1.3451000e-01 /
CHEB / -6.5071000e-01 6.9080000e-01 1.6686000e-01 /
CHEB / -2.6254000e+00 7.4430000e-02 2.0501000e-03 /
CHEB / -1.2179000e+00 -8.1957000e-02 -2.5739000e-02 /
CHEB / -5.4175000e-01 -3.2031000e-02 -9.9389000e-03 /

C4H7O-13+O2(+m)=C3H5O2J(54)+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #98 (C4H7O3J(5))   deltaHrxn(T=298K) = -
2.629337428459827 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -1.9497000e+00 -1.2370000e-02 -1.0317000e-02 /
CHEB / 1.0723000e+01 1.7822000e-02 1.4835000e-02 /
CHEB / 1.5736000e-01 -5.0305000e-03 -4.1442000e-03 /
CHEB / -9.4478000e-03 -1.5034000e-03 -1.2770000e-03 /
CHEB / -6.2741000e-02 1.0337000e-03 8.5453000e-04 /

C4H6O3(3)+H(+m)=C4H7O3J(5)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -32.89597013656652
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2846000e+01 7.2093000e+00 4.2779000e-02 /
CHEB / 1.1348000e+00 -1.3667000e-01 5.3841000e-01 /
CHEB / -3.0619000e+00 -6.1718000e-01 1.7459000e-01 /
CHEB / -1.3938000e+00 -4.7813000e-01 1.8326000e-02 /
CHEB / -5.1784000e-01 -1.5083000e-01 -2.9038000e-02 /

C4H6O3(3)+H(+m)=C4H7O3J(6)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) CO/H/Nd_O     H_rad        deltaHrxn(T=298K) = -
17.037718359735354 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6002000e-01 4.1155000e+00 1.6550000e-01 /
CHEB / -1.0486000e+00 3.1825000e-02 3.6894000e-02 /
CHEB / -2.4007000e+00 -1.1956000e-01 7.5186000e-03 /
CHEB / -1.0855000e+00 -9.5296000e-02 -3.1388000e-02 /
CHEB / -4.9251000e-01 -2.4108000e-02 -1.6126000e-02 /

C4H6O3(3)+H(+m)=C4H7O-13+O2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -11.87863830988175
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.5935000e-01 -1.6456000e-02 -1.2584000e-02 /
CHEB / 8.4376000e+00 2.2364000e-02 1.7285000e-02 /
CHEB / 5.2661000e-01 -5.4107000e-03 -4.4236000e-03 /
CHEB / 7.5510000e-02 -1.0557000e-03 -7.4303000e-04 /
CHEB / -2.9613000e-02 5.4209000e-04 4.7108000e-04 /

C4H6O3(3)+H(+m)=C3H5O2J(54)+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #98 (C4H7O3J(5))   deltaHrxn(T=298K) = -
14.507975738341575 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0083000e+00 -1.1352000e-02 -9.1948000e-03 /
CHEB / 3.1579000e+00 1.5420000e-02 1.2482000e-02 /
CHEB / -9.4772000e-02 -2.7442000e-03 -2.2190000e-03 /
CHEB / -6.6907000e-02 -2.4640000e-03 -1.9746000e-03 /
CHEB / -5.6934000e-02 9.1146000e-04 7.1555000e-04 /

CH2CHCHCHOH+HO2(+m)=C4H7O3J(5)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -9.768962974905445
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7005000e+00 2.4175000e+00 -4.1257000e-01 /
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CHEB / 1.2265000e+00 1.0346000e+00 2.9779000e-01 /
CHEB / -3.3215000e+00 6.0300000e-02 8.6882000e-02 /
CHEB / -1.5542000e+00 -2.3735000e-01 -2.4201000e-02 /
CHEB / -5.5130000e-01 -1.4529000e-01 -3.9148000e-02 /

C4H7O3J(6)(+m)=CH2CHCHCHOH+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -6.0892888019257185
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5270000e+01 5.0690000e+00 6.5389000e-01 /
CHEB / 8.7922000e+00 1.0760000e-01 -6.6198000e-02 /
CHEB / -1.9900000e+00 -2.1030000e-01 -4.3280000e-02 /
CHEB / -9.5957000e-01 -1.3177000e-01 -3.7525000e-02 /
CHEB / -4.6000000e-01 -2.3595000e-02 -4.5629000e-03 /

C4H7O-13+O2(+m)=CH2CHCHCHOH+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -11.248368851779325
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0871000e+00 -3.9024000e-01 -1.6369000e-01 /
CHEB / 3.5013000e+00 5.0521000e-01 1.9574000e-01 /
CHEB / 4.1450000e-02 -6.1744000e-02 1.9849000e-03 /
CHEB / -1.9349000e-02 -6.8539000e-02 -3.5280000e-02 /
CHEB / -9.8069000e-03 -2.6415000e-03 -1.0424000e-02 /

C3H5O2J(54)+CH2O(+m)=CH2CHCHCHOH+HO2(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #98 (C4H7O3J(5))   deltaHrxn(T=298K) = -
8.619031423319498 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.1793000e+00 -2.8075000e-02 -2.0165000e-02 /
CHEB / 1.2788000e+01 3.7169000e-02 2.6716000e-02 /
CHEB / 4.8677000e-01 -6.7456000e-03 -4.8515000e-03 /
CHEB / 7.5968000e-02 -3.5394000e-03 -2.5786000e-03 /
CHEB / -3.6736000e-02 7.6775000e-04 5.6560000e-04 /

C4H6O3(3)+H(+m)=CH2CHCHCHOH+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #98 (C4H7O3J(5))  deltaHrxn(T=298K) = -23.127007161661073
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1605000e+00 -2.8718000e-02 -2.0415000e-02 /
CHEB / 9.5206000e+00 3.8271000e-02 2.7250000e-02 /
CHEB / 8.2307000e-01 -7.9616000e-03 -5.7140000e-03 /
CHEB / 1.6373000e-01 -2.4520000e-03 -1.7554000e-03 /
CHEB / -3.0130000e-03 5.3998000e-04 4.0802000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H5O2J(54) 21.86 78.59 23.19 28.36 32.19 35.33 39.81 42.82 47.49
      null
```

```
!     aC3H5O2     22.49 81.97 21.44 25.44 28.86 31.9  36.69 40.64 46.36
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!Here are the path reactions and their high-P limit kinetics:
!     C3H4O+OH=C3H5O2J(54)    2.3501400e+11      0.30815
4.9629937e+03
!     aC3H5O2=C3H5O2J(54)     3.4152599e+09      1.20000
3.8255000e+04

C3H5O2J(54)(+m)=C3H4O+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3334 (C3H5O2J(54))     deltaHrxn(T=298K) = -
32.85691952850495 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.4273000e+00 2.0000000e+00 -1.2601000e-07 /
CHEB / -2.9568000e-01 -3.5373000e-07 -2.4622000e-07 /
CHEB / -7.7693000e-02 -3.2954000e-07 -2.2938000e-07 /
CHEB / -2.7218000e-02 -2.9164000e-07 -2.0301000e-07 /
CHEB / -1.0717000e-02 -2.4309000e-07 -1.6921000e-07 /

C3H5O2J(54)(+m)=aC3H5O2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3334 (C3H5O2J(54))     deltaHrxn(T=298K) =
0.6301227263116829 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8150000e+01 2.0000000e+00 -1.2595000e-07 /
CHEB / 2.2154000e+01 -3.5357000e-07 -2.4611000e-07 /
CHEB / 9.7479000e-02 -3.2939000e-07 -2.2928000e-07 /
CHEB / 3.4125000e-02 -2.9151000e-07 -2.0291000e-07 /
CHEB / 1.3410000e-02 -2.4297000e-07 -1.6913000e-07 /

C3H4O+OH(+m)=aC3H5O2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3334 (C3H5O2J(54))     deltaHrxn(T=298K) =
33.487042254816636 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7377000e+01 -1.8095000e-07 -1.2595000e-07 /
CHEB / 2.4313000e+01 -3.5357000e-07 -2.4611000e-07 /
CHEB / 2.2684000e-01 -3.2939000e-07 -2.2928000e-07 /
CHEB / 1.0603000e-01 -2.9151000e-07 -2.0291000e-07 /
CHEB / 4.8095000e-02 -2.4297000e-07 -1.6913000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H5O3J(3)  -5.85 95.97 27.82 33.27 37.81 41.26 46.91 51.16 55.18
      null
```

```
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     HCO              10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     CH2CHCHCHO  7.91  74.22 21.64 26.87 31.0  34.29 39.32 42.77 46.7
      null
!     O2               0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     aC3H5O2     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67 46.07
!     CO               -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     HO2              3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H5O2J(13) -6.19 86.99 24.08 29.28 33.8  37.19 42.8  46.53 49.88
      null
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     CH2CHCHCHO+O2=C4H5O3J(3)      3.7700000e+12      0.00000
0.0000000e+00
!     aC3H5O2+CO=C4H5O3J(3)   7.6600000e+05      2.07000
8.2200000e+04
!     C4H5O2J(13)+O=C4H5O3J(3)      1.0000000e+13      0.00000
0.0000000e+00

CH2CHCHCHO+O2(+m)=C4H5O3J(3)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3)) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/TwoDe     O2_birad           deltaHrxn(T=298K) = -
14.438468292781666 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0069000e+00 1.3290000e+00 -1.4238000e-01 /
CHEB / -5.7834000e+00 8.2787000e-01 1.5967000e-01 /
CHEB / -2.9797000e+00 -1.7474000e-02 2.0542000e-02 /
CHEB / -1.1568000e+00 -1.7122000e-01 -3.4641000e-02 /
CHEB / -3.4375000e-01 -2.2095000e-02 -1.7626000e-02 /

C4H5O3J(3)(+m)=aC3H5O2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3))   deltaHrxn(T=298K) = 3.4996531744569452
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7790000e+01 6.7497000e+00 1.5911000e+00 /
CHEB / 2.2729000e+01 -3.6513000e-01 -4.8179000e-02 /
CHEB / -3.0959000e+00 -4.0138000e-01 -7.4860000e-02 /
CHEB / -1.1361000e+00 -2.0931000e-01 -5.2420000e-02 /
CHEB / -3.2987000e-01 -1.4602000e-02 -1.7652000e-02 /

CH2CHCHCHO+O2(+m)=aC3H5O2+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3))   deltaHrxn(T=298K) = -10.93881511832472
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5640000e+01 3.2913000e-06 2.2910000e-06 /
CHEB / 2.4260000e+01 2.1841000e-06 1.5203000e-06 /
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CHEB / 6.6809000e-02 -1.5946000e-07 -1.1101000e-07 /
CHEB / 6.4021000e-03 -7.4218000e-07 -5.1661000e-07 /
CHEB / -1.0061000e-02 -6.5013000e-07 -4.5253000e-07 /

C4H5O2J(13)+O(+m)=C4H5O3J(3)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3)) High-P Limit: Oa_R_Recombination estimate:
(Average:) O_rad/NonDe     Oa       deltaHrxn(T=298K) = -
59.293842487192784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9444000e+00 6.2262000e+00 1.2404000e+00 /
CHEB / -6.8222000e+00 -3.4661000e-01 -3.3194000e-02 /
CHEB / -3.1018000e+00 -3.8043000e-01 -6.0266000e-02 /
CHEB / -1.1247000e+00 -2.0471000e-01 -4.9297000e-02 /
CHEB / -3.1937000e-01 -1.4932000e-02 -1.7860000e-02 /

C4H5O2J(13)+O(+m)=CH2CHCHCHO+O2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3))   deltaHrxn(T=298K) = -44.85537419441112
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3845000e+01 3.0490000e-06 2.1201000e-06 /
CHEB / -7.3847000e-01 1.9954000e-06 1.3918000e-06 /
CHEB / -2.7875000e-02 -2.5292000e-07 -1.7659000e-07 /
CHEB / -1.4670000e-02 -7.4084000e-07 -5.1590000e-07 /
CHEB / -1.0756000e-02 -5.8083000e-07 -4.0409000e-07 /

C4H5O2J(13)+O(+m)=aC3H5O2+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4 (C4H5O3J(3))   deltaHrxn(T=298K) = -55.79418931273584
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4335000e+00 -1.2925000e-03 -8.9917000e-04 /
CHEB / 1.0519000e+01 1.2983000e-03 9.0310000e-04 /
CHEB / 6.8358000e-01 1.4849000e-04 1.0341000e-04 /
CHEB / 2.2620000e-01 -1.0305000e-04 -7.1657000e-05 /
CHEB / 6.4192000e-02 -5.3551000e-05 -3.7274000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     iC4H5OJ(15) 8.76  72.88 22.52 27.78 31.88 35.05 39.89 43.1  46.9
      null
!     H2CCCO      40.46 32.23 9.0   10.76 12.21 13.5  15.37 16.77 18.89
      null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     H2CCCO+CH3=iC4H5OJ(14)  1.9263655e+11      0.04067
9.2900000e+03
!     iC4H5OJ(15)=iC4H5OJ(14) 2.0320555e+08      1.13906
3.4790987e+04
!     sC3H5+CO=iC4H5OJ(14)    1.5100000e+11      0.00000
4.8100000e+03

H2CCCO+CH3(+m)=iC4H5OJ(14)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ca_Ck     C_methyl         deltaHrxn(T=298K) = -
71.70348383950763 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.3848000e+00 6.3442000e+00 8.5005000e-01 /
CHEB / 1.9171000e+00 1.3831000e+00 2.0959000e-01 /
CHEB / -1.3192000e+00 3.2756000e-01 6.8701000e-04 /
CHEB / -6.7882000e-01 4.6423000e-02 -3.1949000e-02 /
CHEB / -3.3596000e-01 -2.9975000e-02 -2.7839000e-02 /

sC3H5+CO(+m)=iC4H5OJ(14)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14)) High-P Limit: R_Addition_COm estimate:
(Average:) Cd_rad/NonDe     COm           deltaHrxn(T=298K) = -
31.566845001153446 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3218000e+00 9.3204000e-01 -1.2520000e-01 /
CHEB / -1.4768000e+00 8.5342000e-01 8.9446000e-02 /
CHEB / -1.5762000e+00 3.3010000e-01 3.3608000e-02 /
CHEB / -8.3498000e-01 6.5241000e-03 1.7027000e-02 /
CHEB / -4.2195000e-01 -6.0643000e-02 -1.0131000e-04 /

H2CCCO+CH3(+m)=sC3H5+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14))     deltaHrxn(T=298K) = -
40.13663883835417 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8530000e+00 3.9298000e-07 2.7353000e-07 /
CHEB / 2.9690000e+00 7.5873000e-07 5.2811000e-07 /
CHEB / 9.1611000e-04 6.8201000e-07 4.7472000e-07 /
CHEB / 3.5056000e-02 5.7036000e-07 3.9701000e-07 /
CHEB / 1.2562000e-02 4.4273000e-07 3.0817000e-07 /

iC4H5OJ(14)(+m)=iC4H5OJ(15)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14))     deltaHrxn(T=298K) =
5.199565657106797 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2605000e+00 1.2837000e+00 -2.2874000e-01 /
CHEB / 1.1088000e+01 7.4449000e-01 1.8630000e-01 /
CHEB / -1.4216000e+00 3.4238000e-01 2.6314000e-02 /
CHEB / -7.7800000e-01 8.1379000e-03 3.6921000e-04 /
CHEB / -3.9431000e-01 -6.5733000e-02 -2.0508000e-03 /
```

```
H2CCCO+CH3(+m)=iC4H5OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14))     deltaHrxn(T=298K) = -
66.50391818240082 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.6328000e+00 -3.1015000e-05 -2.1603000e-05 /
CHEB / 5.0140000e+00 7.6428000e-06 5.3185000e-06 /
CHEB / 5.4906000e-01 1.8640000e-05 1.2988000e-05 /
CHEB / 2.2772000e-01 6.8087000e-06 4.7462000e-06 /
CHEB / 8.8311000e-02 3.2915000e-07 2.2849000e-07 /

sC3H5+CO(+m)=iC4H5OJ(15)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #4277 (iC4H5OJ(14))     deltaHrxn(T=298K) = -
26.36727934404665 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7365000e+00 -5.1026000e-01 -1.4461000e-01 /
CHEB / 4.1433000e+00 6.0381000e-01 1.4680000e-01 /
CHEB / 4.9498000e-01 -2.6792000e-02 2.0614000e-02 /
CHEB / 1.4040000e-01 -6.1351000e-02 -9.2526000e-03 /
CHEB / 7.2839000e-02 -1.0122000e-02 -1.2939000e-02 /

!PDepNetwork C12H10
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C12H10      43.52 92.93 39.97 52.98 64.39 73.81 86.86 96.0  108.42
       !Burcat 30SEPT2010
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C6H5             80.61 68.37 18.54 25.1  30.94 35.75 42.22 46.78
      52.97  !Burcat 07-Jan-2011
!Here are the path reactions and their high-P limit kinetics:
!     C6H5+C6H5=C12H10        2.000e+13    0.00        0.00

C6H5+C6H5(+m)=C12H10(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C12H10) High-P Limit: R_Recombination Primary Kinetic
Library: MRH      deltaHrxn(T=298K) = -117.68863630356927 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3348000e+01 8.2524000e-02 -2.6633000e-02 /
CHEB / -2.0549000e-01 1.5809000e-01 -5.0463000e-02 /
CHEB / -1.0169000e-01 1.3876000e-01 -4.2770000e-02 /
CHEB / -8.4853000e-02 1.1123000e-01 -3.2091000e-02 /
CHEB / -6.1829000e-02 8.0927000e-02 -2.0890000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H5OJ(15) 8.76  72.88 22.52 27.78 31.88 35.05 39.89 43.1  46.9
      null
```

```
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     aC3H4             46.72 58.47 14.1  17.12 19.72 22.0  25.44 28.04
      32.08 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     aC3H5             40.75 62.05 14.83 18.67 21.94 24.67 28.9  32.03
      36.9  null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!Here are the path reactions and their high-P limit kinetics:
!     aC3H4+HCO=iC4H5OJ(15)   5.2000000e+11      0.00000
6.5600000e+03
!     aC3H5+CO=iC4H5OJ(15)    5.9198482e+04      2.36750
7.2970000e+04
!     iC4H5OJ(15)=iC4H5OJ(14) 2.0320555e+08      1.13906
3.4790987e+04

aC3H4+HCO(+m)=iC4H5OJ(15)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #37 (iC4H5OJ(15)) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ca_Cd/H2     CO_pri_rad          deltaHrxn(T=298K)
= -48.355050202410325 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0909000e+00 7.3860000e-01 -1.5769000e-01 /
CHEB / 5.5488000e-01 8.5532000e-01 -3.9559000e-02 /
CHEB / -5.3210000e-01 3.0624000e-01 6.5840000e-02 /
CHEB / -1.8827000e-01 2.4928000e-02 5.8326000e-02 /
CHEB / -6.1881000e-02 -3.0799000e-02 1.8380000e-02 /

iC4H5OJ(15)(+m)=aC3H5+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #37 (iC4H5OJ(15)) deltaHrxn(T=298K) = 5.569465920567488
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9472000e+01 1.8428000e+00 -9.6807000e-02 /
CHEB / 2.5895000e+01 8.1182000e-02 5.0282000e-02 /
CHEB / -3.7778000e-01 5.5503000e-02 3.1533000e-02 /
CHEB / -8.9487000e-02 -4.9415000e-03 -2.5191000e-03 /
CHEB / -2.8050000e-02 -7.6195000e-03 -3.7301000e-03 /

aC3H4+HCO(+m)=aC3H5+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #37 (iC4H5OJ(15)) deltaHrxn(T=298K) = -42.78558428184284
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1071000e+00 -1.2548000e-01 -7.8150000e-02 /
CHEB / 1.0806000e+01 9.9142000e-02 6.1298000e-02 /
CHEB / 2.4935000e-01 3.7300000e-02 2.1807000e-02 /
CHEB / 5.8027000e-02 -1.6617000e-02 -9.1418000e-03 /
CHEB / 5.1519000e-03 -7.8199000e-03 -4.2717000e-03 /

aC3H4+HCO(+m)=iC4H5OJ(14)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #37 (iC4H5OJ(15)) deltaHrxn(T=298K) = -53.55461585951712
kcal/mol
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TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0544000e+00 -1.1627000e+00 -1.4747000e-01 /
CHEB / 2.6139000e+00 9.3874000e-01 -5.8192000e-03 /
CHEB / 4.4056000e-02 2.6666000e-01 8.5707000e-02 /
CHEB / -8.9966000e-02 -2.9490000e-02 5.1005000e-02 /
CHEB / -3.4912000e-02 -5.3233000e-02 2.8669000e-03 /

aC3H5+CO(+m)=iC4H5OJ(14)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #37 (iC4H5OJ(15)) deltaHrxn(T=298K) = -10.769031577674285
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0110000e+01 -1.4124000e-01 -8.7427000e-02 /
CHEB / 2.6369000e+01 9.3343000e-02 5.7642000e-02 /
CHEB / 3.6393000e-01 4.9169000e-02 2.8318000e-02 /
CHEB / 9.8959000e-02 -1.1150000e-02 -5.9434000e-03 /
CHEB / 2.8609000e-02 -9.0437000e-03 -4.6804000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H7-2            21.02 69.01 16.58 20.27 24.03 27.49 33.13 37.52
      44.42 null
!     HCOOH       -90.2 59.4  10.83 12.87 14.62 15.98 18.4  20.0  20.0
      null
!     C4H8O-i3    -51.2 79.65 23.57 29.46 34.96 39.45 46.7  51.93 57.55
      null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H9Oi3     -25.01      84.17 26.86 33.02 38.34 42.86 49.96 55.22
      61.63 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H8O-i3+OH(+m)=C3H7-2+HCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #70 (spc1)  deltaHrxn(T=298K) = -27.296784180264865 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0568000e+01 -5.8856000e-05 -4.0964000e-05 /
CHEB / 1.4563000e+00 -9.1500000e-05 -6.3682000e-05 /
CHEB / 4.7764000e-02 -7.1272000e-05 -4.9603000e-05 /
CHEB / 2.5295000e-02 -5.3398000e-05 -3.7162000e-05 /
CHEB / 5.3038000e-03 -3.4691000e-05 -2.4143000e-05 /

C4H9Oi3+O(+m)=C3H7-2+HCOOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #70 (spc1)  deltaHrxn(T=298K) = -103.70895411151628 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / 1.3575000e+01 -3.0020000e-05 -2.0895000e-05 /
CHEB / -5.7193000e-01 -5.1001000e-05 -3.5498000e-05 /
CHEB / -6.4046000e-02 -3.9990000e-05 -2.7834000e-05 /
CHEB / -2.4574000e-02 -2.8894000e-05 -2.0110000e-05 /
CHEB / -2.0404000e-02 -1.8283000e-05 -1.2725000e-05 /

C4H9Oi3+O(+m)=C4H8O-i3+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #70 (spc1)  deltaHrxn(T=298K) = -76.4121699312514 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1783000e+01 -2.8477000e-05 -1.9821000e-05 /
CHEB / 6.7023000e-01 -4.8066000e-05 -3.3455000e-05 /
CHEB / 3.6241000e-01 -3.7442000e-05 -2.6061000e-05 /
CHEB / 1.3727000e-01 -2.6856000e-05 -1.8692000e-05 /
CHEB / 4.1675000e-02 -1.6780000e-05 -1.1679000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2CCCH3[OH] -38.81      72.62 19.18 23.26 26.77 29.82 34.95 38.72
      44.37 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

C4H8O-i1+OH(+m)=H2CCCH3[OH]+CH2OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #93 (spc2)   deltaHrxn(T=298K) = -13.4583191897279
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1424000e+01 -9.0422000e-01 -1.1393000e-01 /
CHEB / 7.0349000e-01 1.0310000e+00 6.7829000e-02 /
CHEB / -2.9643000e-01 4.7782000e-02 8.7449000e-02 /
CHEB / -1.9523000e-01 -1.5218000e-01 -1.0551000e-02 /
CHEB / -5.0596000e-02 -6.2697000e-02 -3.3195000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     HCOOH       -90.2 59.4  10.83 12.87 14.62 15.98 18.4  20.0  20.0
      null
```

```
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-13+OH(+m)=sC3H5+HCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (spc3) deltaHrxn(T=298K) = -10.628352669667976 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1322000e+01 -4.1500000e-03 -2.8727000e-03 /
CHEB / 8.6820000e-01 5.6522000e-03 3.9116000e-03 /
CHEB / 6.9275000e-02 -1.2406000e-03 -8.5820000e-04 /
CHEB / 4.6059000e-02 -7.0274000e-04 -4.8542000e-04 /
CHEB / 2.2687000e-02 3.7355000e-04 2.5762000e-04 /

tSPC(110)+OH(+m)=sC3H5+HCOOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (spc3) deltaHrxn(T=298K) = -64.03295194764866 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3475000e+01 -2.9736000e-05 -2.0698000e-05 /
CHEB / -7.0451000e-01 1.0985000e-05 7.6461000e-06 /
CHEB / -3.2226000e-02 -2.7454000e-06 -1.9110000e-06 /
CHEB / -1.7873000e-03 -6.8166000e-06 -4.7448000e-06 /
CHEB / -4.7526000e-03 -3.2282000e-06 -2.2470000e-06 /

iC4H7OJ(15)+O(+m)=sC3H5+HCOOH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (spc3) deltaHrxn(T=298K) = -78.36166671561466 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3367000e+01 -2.0895000e-05 -1.4545000e-05 /
CHEB / -3.2893000e-01 4.5111000e-06 3.1400000e-06 /
CHEB / -1.2833000e-02 -3.1911000e-06 -2.2212000e-06 /
CHEB / -1.3153000e-03 -5.4630000e-06 -3.8026000e-06 /
CHEB / -3.1055000e-03 -2.8631000e-06 -1.9929000e-06 /

iC4H7OJ(15)+O(+m)=C4H6Oi-13+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (spc3) deltaHrxn(T=298K) = -67.73331404594668 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1748000e+01 -2.0776000e-05 -1.4462000e-05 /
CHEB / 1.2775000e-01 4.6558000e-06 3.2407000e-06 /
CHEB / 1.3135000e-01 -3.1202000e-06 -2.1718000e-06 /
CHEB / 5.2970000e-02 -5.4073000e-06 -3.7638000e-06 /
CHEB / 1.9024000e-02 -2.8307000e-06 -1.9703000e-06 /
```

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iC4H7OJ(15)+O(+m)=tSPC(110)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (spc3) deltaHrxn(T=298K) = -14.328714767966007 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5863000e+00 -1.8902000e-05 -1.3157000e-05 /
CHEB / 2.2031000e+00 5.8671000e-06 4.0839000e-06 /
CHEB / 8.8679000e-01 -2.8583000e-06 -1.9895000e-06 /
CHEB / 2.8781000e-01 -4.8441000e-06 -3.3718000e-06 /
CHEB / 9.5017000e-02 -2.5295000e-06 -1.7607000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     iC4H7OJ(51) -12.13      83.88 23.19 27.95 32.44 36.36 42.62 47.3
      54.55  !MRH CBS-QB3 w/1DHR corrections
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     OCOOH       -24.73      72.56 16.22 18.34 19.59 20.32 21.26 21.61
      21.32 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     tSPC(1416)  -61.04      85.71 24.27 29.59 33.62 36.68 40.98 43.84
      47.56 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

O2+iC4H7OJ(51)(+m)=OCOOH+C3H6(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(335)) deltaHrxn(T=298K) = -7.039446826677076
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.0447000e+00 -1.1261000e+00 -2.6976000e-01 /
CHEB / 8.8747000e-01 1.3366000e+00 2.6055000e-01 /
CHEB / -4.2798000e-01 -3.5545000e-02 7.2749000e-02 /
CHEB / -2.1472000e-01 -1.5412000e-01 -3.5977000e-02 /
CHEB / -5.0641000e-02 -5.9770000e-02 -3.3312000e-02 /

O2+iC4H7OJ(51)(+m)=tSPC(1416)+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(335))  deltaHrxn(T=298K) = -
14.338990643431934 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
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CHEB / 5    3 /
CHEB / 1.0441000e+01 -1.3244000e+00 -2.6957000e-01 /
CHEB / 4.1089000e-01 1.5520000e+00 2.3568000e-01 /
CHEB / -4.7171000e-01 -4.3990000e-03 1.0168000e-01 /
CHEB / -2.4767000e-01 -1.8855000e-01 -2.7020000e-02 /
CHEB / -5.5978000e-02 -8.4742000e-02 -4.2320000e-02 /

OCOOH+C3H6(+m)=tSPC(1416)+CH3(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(335)) deltaHrxn(T=298K) = -7.299543816754856
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7314000e+00 -4.5290000e-01 -1.4653000e-01 /
CHEB / 2.6144000e+00 5.9990000e-01 1.7386000e-01 /
CHEB / -8.6971000e-02 -9.5680000e-02 5.4150000e-03 /
CHEB / -1.1696000e-02 -7.1884000e-02 -3.4732000e-02 /
CHEB / 2.6489000e-02 2.3689000e-03 -9.3318000e-03 /

O2+iC4H7OJ(51)(+m)=C4H6Oi-12+HO2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(335))  deltaHrxn(T=298K) = -
7.283264221206627 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0879000e+01 -8.9658000e-01 -1.4621000e-01 /
CHEB / 5.8300000e-01 9.9550000e-01 9.0810000e-02 /
CHEB / -1.9020000e-01 7.7094000e-02 1.0343000e-01 /
CHEB / -1.4946000e-01 -1.3790000e-01 -8.8446000e-03 /
CHEB / -3.4158000e-02 -7.2868000e-02 -3.9220000e-02 /

C4H6Oi-12+HO2(+m)=OCOOH+C3H6(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #2 (C4H7O3J(335)) deltaHrxn(T=298K) = 0.2438173945295512
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4192000e+00 -1.4222000e+00 -2.7405000e-01 /
CHEB / 3.0304000e+00 1.6102000e+00 2.3413000e-01 /
CHEB / -2.0101000e-01 6.3326000e-02 1.0117000e-01 /
CHEB / -3.6018000e-02 -1.9644000e-01 -1.7132000e-02 /
CHEB / 7.6887000e-02 -1.0042000e-01 -3.9909000e-02 /

C4H6Oi-12+HO2(+m)=tSPC(1416)+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #2 (C4H7O3J(335))  deltaHrxn(T=298K) = -
7.055726422225312 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.1994000e+00 -1.8232000e+00 -1.9929000e-01 /
CHEB / 2.1463000e+00 1.9817000e+00 1.1217000e-01 /
CHEB / -2.6061000e-01 1.7701000e-01 1.3196000e-01 /
CHEB / -1.1079000e-01 -2.3099000e-01 8.3547000e-03 /
CHEB / 7.2179000e-02 -1.5058000e-01 -3.1722000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
```

```
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HCO               10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C3H5OJ(12)        -4.96 71.27 18.06 21.58 24.93 27.85 32.53 36.02
      41.39
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     iC4H7OJ(48) -0.88 82.81 25.44 29.81 33.87 37.43 43.22 47.64 54.64
!MRH CBS-QB3 w/1DHR corrections
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C3H7O2      -8.38 83.49 23.02 28.24 32.94 36.92 43.11 47.67 54.73
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H4O             -14.2 65.35 16.87 20.41 23.49 26.1  30.14 33.04
      37.3
!     CH2CH2CH2OOH      7.26  88.49 25.27 30.39 34.78 38.41 43.99 48.1
      54.53
!     C3H4O-enone       -13.82      68.58 16.45 19.54 22.36 24.81 28.75
      31.71 36.31
!Here are the path reactions and their high-P limit kinetics:

C3H5OJ(12)+nSPC(102)(+m)=iC4H7OJ(48)+O2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -46.34553221614104 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2708000e+01 -1.1459000e-03 -9.4600000e-04 /
CHEB / -7.3737000e-01 1.3998000e-03 1.1727000e-03 /
CHEB / -2.2643000e-01 -9.6852000e-05 -9.9689000e-05 /
CHEB / -1.2984000e-01 -1.9006000e-04 -1.6164000e-04 /
CHEB / -9.1593000e-02 1.4340000e-05 1.7206000e-05 /
```

```
C3H5OJ(12)+nSPC(102)(+m)=C3H7O2+CO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
80.96163964262749 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.0698000e+00 -1.6036000e-02 -1.0993000e-02 /
CHEB / 4.0763000e+00 2.0187000e-02 1.3805000e-02 /
CHEB / 9.4087000e-01 -2.3319000e-03 -1.5459000e-03 /
CHEB / 1.6858000e-01 -2.1974000e-03 -1.5171000e-03 /
CHEB / -2.7407000e-02 1.3721000e-05 -2.8956000e-06 /

iC4H7OJ(48)+O2(+m)=C3H7O2+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
34.61610742648645 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0185000e+00 -1.1459000e-03 -9.4600000e-04 /
CHEB / 1.6109000e+01 1.3998000e-03 1.1727000e-03 /
CHEB / 7.8290000e-02 -9.6852000e-05 -9.9689000e-05 /
CHEB / -6.0247000e-03 -1.9006000e-04 -1.6164000e-04 /
CHEB / -3.7965000e-02 1.4340000e-05 1.7206000e-05 /

C3H5OJ(12)+nSPC(102)(+m)=tSPC(213)+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
39.6467418915286 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2788000e+00 -1.6678000e-03 -1.3739000e-03 /
CHEB / 1.2805000e+00 2.2123000e-03 1.8123000e-03 /
CHEB / 1.7363000e-01 -3.6484000e-04 -2.7927000e-04 /
CHEB / -4.7993000e-02 -2.2953000e-04 -2.0781000e-04 /
CHEB / -7.9842000e-02 4.3602000e-05 3.6145000e-05 /

tSPC(213)+H(+m)=iC4H7OJ(48)+O2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
6.698790324612439 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0677000e+01 -9.6694000e-01 -3.1668000e-01 /
CHEB / 1.3096000e+00 1.1660000e+00 3.2399000e-01 /
CHEB / -3.2239000e-01 -4.3161000e-02 7.4847000e-02 /
CHEB / -2.1789000e-01 -1.5491000e-01 -6.3866000e-02 /
CHEB / -8.4539000e-02 -3.9539000e-02 -3.4697000e-02 /

tSPC(213)+H(+m)=C3H7O2+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
41.31489775109889 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0092000e+00 -1.6678000e-03 -1.3739000e-03 /
CHEB / 1.5183000e+01 2.2123000e-03 1.8123000e-03 /
CHEB / 1.7278000e-01 -3.6484000e-04 -2.7927000e-04 /
CHEB / -9.5643000e-03 -2.2953000e-04 -2.0781000e-04 /
CHEB / -4.0501000e-02 4.3602000e-05 3.6145000e-05 /
```

```
C3H5OJ(12)+nSPC(102)(+m)=HO2+C4H6Oi-13(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -70.41292913957798 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1321000e+01 3.8704000e-03 2.6413000e-03 /
CHEB / -1.5424000e-01 -4.0949000e-03 -2.7645000e-03 /
CHEB / -1.2245000e-01 -4.7696000e-04 -3.6447000e-04 /
CHEB / -9.7837000e-02 5.0006000e-04 3.3483000e-04 /
CHEB / -7.5104000e-02 2.9374000e-04 2.1745000e-04 /

iC4H7OJ(48)+O2(+m)=HO2+C4H6Oi-13(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
24.06739692343694 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1243000e+01 -1.0328000e+00 -9.4238000e-02 /
CHEB / 5.9396000e-01 1.1055000e+00 2.7895000e-02 /
CHEB / -2.2307000e-01 1.5156000e-01 9.5423000e-02 /
CHEB / -1.9356000e-01 -1.6250000e-01 1.3286000e-02 /
CHEB / -7.5039000e-02 -1.0763000e-01 -3.2937000e-02 /

HO2+C4H6Oi-13(+m)=C3H7O2+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
10.548710503049511 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8307000e+01 3.8704000e-03 2.6413000e-03 /
CHEB / 2.4844000e+01 -4.0949000e-03 -2.7645000e-03 /
CHEB / 1.5850000e-01 -4.7696000e-04 -3.6447000e-04 /
CHEB / 2.6170000e-02 5.0006000e-04 3.3483000e-04 /
CHEB / -9.9699000e-03 2.9374000e-04 2.1745000e-04 /

tSPC(213)+H(+m)=HO2+C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
30.76618724804938 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3508000e+01 -1.1000000e-02 -8.8025000e-03 /
CHEB / -4.3189000e-01 1.3233000e-02 1.0756000e-02 /
CHEB / -1.8446000e-01 -1.0855000e-04 -3.1193000e-04 /
CHEB / -1.2464000e-01 -2.4175000e-03 -1.9884000e-03 /
CHEB / -8.8324000e-02 -1.4280000e-04 -1.1241000e-05 /

C3H5OJ(12)+nSPC(102)(+m)=HO2+tSPC(110)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -17.008329861597293 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0407000e+00 -1.8681000e-02 -1.2888000e-02 /
CHEB / 1.7341000e+00 2.2126000e-02 1.5240000e-02 /
CHEB / 4.1573000e-01 -6.9835000e-04 -4.4491000e-04 /
CHEB / -2.5842000e-02 -2.7742000e-03 -1.9179000e-03 /
CHEB / -1.1028000e-01 -4.8527000e-04 -3.4399000e-04 /
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HO2+tSPC(110)(+m)=iC4H7OJ(48)+O2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
29.337202354543745 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.9054000e+00 -6.0588000e-02 -4.5650000e-02 /
CHEB / 4.0338000e-01 7.7637000e-02 5.7950000e-02 /
CHEB / -9.4030000e-02 -8.4780000e-03 -5.4354000e-03 /
CHEB / -1.6146000e-01 -1.1012000e-02 -8.5514000e-03 /
CHEB / -1.4114000e-01 -2.1175000e-04 -4.6902000e-04 /

HO2+tSPC(110)(+m)=C3H7O2+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
63.9533097810302 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9040000e+00 -1.8681000e-02 -1.2888000e-02 /
CHEB / 8.4786000e+00 2.2126000e-02 1.5240000e-02 /
CHEB / 6.4892000e-01 -6.9835000e-04 -4.4491000e-04 /
CHEB / 6.8556000e-02 -2.7742000e-03 -1.9179000e-03 /
CHEB / -6.5170000e-02 -4.8527000e-04 -3.4399000e-04 /

HO2+tSPC(110)(+m)=tSPC(213)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
22.63841202993131 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0567000e+01 -1.9700000e-03 -1.2566000e-03 /
CHEB / 1.3217000e+00 1.6641000e-03 1.0267000e-03 /
CHEB / 3.6256000e-01 7.6276000e-04 5.1459000e-04 /
CHEB / 1.9094000e-02 -2.0397000e-04 -1.0485000e-04 /
CHEB / -5.3837000e-02 -2.5891000e-04 -1.7120000e-04 /

C3H5OJ(12)+nSPC(102)(+m)=CH2OOH+C3H3OH(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -26.54757118695225 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.5792000e+00 -8.8759000e-02 -5.9652000e-02 /
CHEB / 2.1841000e+00 1.0890000e-01 7.2696000e-02 /
CHEB / 4.2997000e-01 -7.1299000e-03 -4.0300000e-03 /
CHEB / -1.8034000e-02 -1.4606000e-02 -9.9132000e-03 /
CHEB / -9.6855000e-02 -1.5321000e-03 -1.2654000e-03 /

CH2OOH+C3H3OH(+m)=iC4H7OJ(48)+O2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
19.797961029188787 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.2980000e+00 -4.6522000e-01 -2.4646000e-01 /
CHEB / 3.9001000e+00 5.6428000e-01 2.8205000e-01 /
CHEB / -2.0627000e-01 -1.6907000e-02 1.4173000e-02 /
CHEB / -2.4791000e-01 -8.3897000e-02 -4.2422000e-02 /
CHEB / -1.5125000e-01 -2.0130000e-02 -1.9278000e-02 /
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CH2OOH+C3H3OH(+m)=C3H7O2+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
54.414068455675235 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8631000e+00 -8.8759000e-02 -5.9652000e-02 /
CHEB / 1.1995000e+01 1.0890000e-01 7.2696000e-02 /
CHEB / 5.8931000e-01 -7.1299000e-03 -4.0300000e-03 /
CHEB / 6.1401000e-02 -1.4606000e-02 -9.9132000e-03 /
CHEB / -5.1999000e-02 -1.5321000e-03 -1.2654000e-03 /

tSPC(213)+H(+m)=CH2OOH+C3H3OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) =
13.099170704576348 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.6238000e+00 -3.9261000e-01 -1.7891000e-01 /
CHEB / 7.8574000e+00 4.7135000e-01 1.9839000e-01 /
CHEB / -9.0561000e-02 -1.2145000e-02 1.8473000e-02 /
CHEB / -4.9306000e-02 -6.7428000e-02 -3.1485000e-02 /
CHEB / -1.5507000e-03 -1.5965000e-02 -1.5552000e-02 /

CH2OOH+C3H3OH(+m)=HO2+C4H6Oi-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
43.86535795262573 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.4388000e+00 -3.6491000e-01 -1.8555000e-01 /
CHEB / 2.6904000e+00 4.4393000e-01 2.0936000e-01 /
CHEB / -4.0412000e-01 -6.0790000e-03 2.0314000e-02 /
CHEB / -2.8158000e-01 -7.4385000e-02 -3.6558000e-02 /
CHEB / -1.3700000e-01 -2.1820000e-02 -2.0392000e-02 /

HO2+tSPC(110)(+m)=CH2OOH+C3H3OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
9.539241325354958 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.1751000e+00 -2.9054000e-01 -1.3998000e-01 /
CHEB / 3.4378000e+00 3.7120000e-01 1.6911000e-01 /
CHEB / 5.1092000e-01 -4.4723000e-02 -5.6466000e-03 /
CHEB / -7.4813000e-03 -4.4956000e-02 -2.5308000e-02 /
CHEB / -5.5837000e-02 -6.9151000e-04 -4.2493000e-03 /

tSPC(77)+O(+m)=C3H5OJ(12)+nSPC(102)(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
27.52686268970296 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5227000e-01 -5.5618000e-03 -3.8750000e-03 /
CHEB / 3.4057000e+00 5.8833000e-03 4.0996000e-03 /
CHEB / 9.1061000e-01 6.2343000e-04 4.3383000e-04 /
CHEB / 1.8726000e-01 -6.9746000e-04 -4.8632000e-04 /
CHEB / -7.6987000e-03 -3.5759000e-04 -2.4895000e-04 /
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tSPC(77)+O(+m)=iC4H7OJ(48)+O2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
73.87239490584399 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.7034000e+00 2.0438000e-03 1.4363000e-03 /
CHEB / 1.9023000e+00 -1.6658000e-03 -1.1734000e-03 /
CHEB / 2.6777000e-01 -6.1241000e-04 -4.2918000e-04 /
CHEB / -4.2389000e-02 5.0580000e-05 3.7487000e-05 /
CHEB / -7.0479000e-02 1.4350000e-04 1.0114000e-04 /

tSPC(77)+O(+m)=C3H7O2+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
108.48850233233046 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4823000e+00 -5.5618000e-03 -3.8750000e-03 /
CHEB / 4.4902000e+00 5.8833000e-03 4.0996000e-03 /
CHEB / 1.1956000e+00 6.2343000e-04 4.3383000e-04 /
CHEB / 2.8711000e-01 -6.9746000e-04 -4.8632000e-04 /
CHEB / 3.1605000e-02 -3.5759000e-04 -2.4895000e-04 /

tSPC(77)+O(+m)=HO2+C4H6Oi-13(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
97.93979182928095 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.7403000e+00 2.0887000e-03 1.4684000e-03 /
CHEB / 8.1760000e-01 -1.7032000e-03 -1.2002000e-03 /
CHEB / 1.0164000e-01 -6.3451000e-04 -4.4485000e-04 /
CHEB / -5.6698000e-02 4.6245000e-05 3.4574000e-05 /
CHEB / -3.8896000e-02 1.4745000e-04 1.0398000e-04 /

tSPC(77)+O(+m)=HO2+tSPC(110)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
44.535192551300256 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3462000e+00 -1.8646000e-03 -1.3020000e-03 /
CHEB / 2.1109000e+00 1.9275000e-03 1.3464000e-03 /
CHEB / 6.6673000e-01 2.7117000e-04 1.8901000e-04 /
CHEB / 1.7163000e-01 -2.2394000e-04 -1.5671000e-04 /
CHEB / 4.0886000e-02 -1.4244000e-04 -9.9390000e-05 /

tSPC(77)+O(+m)=CH2OOH+C3H3OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
54.074433876655206 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3853000e+00 -1.5365000e-03 -1.0731000e-03 /
CHEB / 1.4503000e+00 1.6163000e-03 1.1293000e-03 /
CHEB / 5.7507000e-01 1.9315000e-04 1.3453000e-04 /
CHEB / 2.1219000e-01 -1.9403000e-04 -1.3582000e-04 /
CHEB / 6.7697000e-02 -1.1222000e-04 -7.8280000e-05 /
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C3H5OJ(12)+nSPC(102)(+m)=C3H4O+CH2OOH(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
45.33553790521339 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.3859000e+00 2.4000000e-03 1.4046000e-03 /
CHEB / 7.0381000e-01 -2.3100000e-03 -1.2657000e-03 /
CHEB / 9.1559000e-03 -4.6684000e-04 -3.5948000e-04 /
CHEB / -8.9912000e-02 1.6157000e-04 5.1799000e-05 /
CHEB / -8.5995000e-02 2.4700000e-04 1.8124000e-04 /

iC4H7OJ(48)+O2(+m)=C3H4O+CH2OOH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) =
1.009994310927647 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5027000e+00 -1.0097000e+00 -3.4512000e-01 /
CHEB / 3.6500000e+00 1.2299000e+00 3.6587000e-01 /
CHEB / -2.2941000e-01 -6.9377000e-02 5.8685000e-02 /
CHEB / -2.0125000e-01 -1.4843000e-01 -6.0531000e-02 /
CHEB / -9.5059000e-02 -4.0660000e-02 -3.5120000e-02 /

C3H4O+CH2OOH(+m)=C3H7O2+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
35.6261017374141 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0978000e+01 2.4000000e-03 1.4046000e-03 /
CHEB / 1.6997000e+01 -2.3100000e-03 -1.2657000e-03 /
CHEB / 1.8837000e-01 -4.6684000e-04 -3.5948000e-04 /
CHEB / -1.9650000e-02 1.6157000e-04 5.1799000e-05 /
CHEB / -4.9874000e-02 2.4700000e-04 1.8124000e-04 /

tSPC(213)+H(+m)=C3H4O+CH2OOH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
5.688796013684794 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0121000e+00 -3.3997000e-01 -1.4701000e-01 /
CHEB / 2.8433000e+00 4.4418000e-01 1.7817000e-01 /
CHEB / 1.1592000e-01 -6.9999000e-02 -5.9841000e-03 /
CHEB / -2.0522000e-02 -4.4723000e-02 -2.7783000e-02 /
CHEB / -2.5976000e-02 1.6452000e-04 -3.9687000e-03 /

C3H4O+CH2OOH(+m)=HO2+C4H6Oi-13(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
25.07739123436459 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1775000e+00 -1.0365000e+00 -3.6093000e-01 /
CHEB / 3.2612000e+00 1.2567000e+00 3.7835000e-01 /
CHEB / -3.1681000e-01 -4.9561000e-02 6.9033000e-02 /
CHEB / -2.3433000e-01 -1.6483000e-01 -6.1762000e-02 /
CHEB / -9.8060000e-02 -5.3114000e-02 -4.2838000e-02 /
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HO2+tSPC(110)(+m)=C3H4O+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
28.327208043616096 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1737000e+00 -8.6861000e-02 -6.5807000e-02 /
CHEB / 2.4417000e+00 1.1136000e-01 8.3797000e-02 /
CHEB / 5.4823000e-01 -1.1800000e-02 -7.9096000e-03 /
CHEB / 8.9528000e-02 -1.6910000e-02 -1.3094000e-02 /
CHEB / -5.2678000e-02 2.4418000e-04 -2.0209000e-04 /

CH2OOH+C3H3OH(+m)=C3H4O+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
18.78796671826114 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -4.7202000e-01 -5.0155000e-01 -2.7265000e-01 /
CHEB / 5.8852000e+00 6.1059000e-01 3.1695000e-01 /
CHEB / 4.1292000e-01 -2.5173000e-02 6.8615000e-03 /
CHEB / 1.1322000e-02 -8.9097000e-02 -4.6584000e-02 /
CHEB / -4.7355000e-02 -1.6880000e-02 -1.7450000e-02 /

tSPC(77)+O(+m)=C3H4O+CH2OOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
72.86240059491635 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7828000e-01 -3.9131000e-04 -2.7423000e-04 /
CHEB / 3.3122000e+00 5.7234000e-04 4.0069000e-04 /
CHEB / 7.8165000e-01 -6.5142000e-05 -4.5469000e-05 /
CHEB / 1.6270000e-01 -1.1513000e-04 -8.0554000e-05 /
CHEB / 1.0362000e-02 -3.1093000e-05 -2.1672000e-05 /

C3H5OJ(12)+nSPC(102)(+m)=CH2CH2CH2OOH+CO(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -65.3235424769822 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0670000e+00 -1.4662000e-02 -1.0119000e-02 /
CHEB / 6.2091000e+00 1.7437000e-02 1.2016000e-02 /
CHEB / 9.5960000e-01 -7.4190000e-04 -4.8535000e-04 /
CHEB / 1.5630000e-01 -2.0432000e-03 -1.4130000e-03 /
CHEB / -3.1129000e-02 -3.4969000e-04 -2.4754000e-04 /

iC4H7OJ(48)+O2(+m)=CH2CH2CH2OOH+CO(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
18.978010260841156 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0689000e+01 1.8776000e-03 1.2984000e-03 /
CHEB / 1.9147000e+01 -1.4949000e-03 -1.0268000e-03 /
CHEB / 1.0646000e-01 -6.9266000e-04 -4.8612000e-04 /
CHEB / -5.9478000e-02 9.4318000e-05 6.1967000e-05 /
CHEB / -7.0860000e-02 1.7853000e-04 1.2621000e-04 /
```

```
C3H7O2+CO(+m)=CH2CH2CH2OOH+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) =
15.638097165645295 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.3100000e+01 -1.4662000e-02 -1.0119000e-02 /
CHEB / 3.4977000e+01 1.7437000e-02 1.2016000e-02 /
CHEB / 1.3044000e+00 -7.4190000e-04 -4.8535000e-04 /
CHEB / 2.8113000e-01 -2.0432000e-03 -1.4130000e-03 /
CHEB / 2.1848000e-02 -3.4969000e-04 -2.4754000e-04 /

tSPC(213)+H(+m)=CH2CH2CH2OOH+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
25.676800585453595 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.0272000e+00 -2.5897000e-04 -1.8132000e-04 /
CHEB / 1.6828000e+01 2.5670000e-04 1.7969000e-04 /
CHEB / 2.1422000e-01 6.3774000e-05 4.4756000e-05 /
CHEB / 5.4855000e-02 -3.8994000e-05 -2.7379000e-05 /
CHEB / 5.0039000e-03 -2.5419000e-05 -1.7822000e-05 /

HO2+C4H6Oi-13(+m)=CH2CH2CH2OOH+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) =
5.0893866625957855 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1850000e+01 3.3049000e-03 2.3424000e-03 /
CHEB / 2.7890000e+01 -2.5637000e-03 -1.8243000e-03 /
CHEB / 2.3593000e-01 -1.4251000e-03 -1.0058000e-03 /
CHEB / -2.4033000e-02 3.1390000e-04 2.2690000e-04 /
CHEB / -4.9488000e-02 3.4159000e-04 2.4289000e-04 /

HO2+tSPC(110)(+m)=CH2CH2CH2OOH+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
48.3152126153849 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.9854000e+00 -3.9876000e-03 -2.7703000e-03 /
CHEB / 1.1498000e+01 4.0372000e-03 2.8034000e-03 /
CHEB / 9.4956000e-01 7.7679000e-04 5.4111000e-04 /
CHEB / 1.7673000e-01 -6.3203000e-04 -4.3855000e-04 /
CHEB / -1.5379000e-02 -2.9398000e-04 -2.0484000e-04 /

CH2OOH+C3H3OH(+m)=CH2CH2CH2OOH+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
38.77597129002994 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1075000e+01 -2.8191000e-02 -1.9886000e-02 /
CHEB / 1.5059000e+01 3.3909000e-02 2.3932000e-02 /
CHEB / 9.1452000e-01 -1.4019000e-03 -1.0010000e-03 /
CHEB / 1.7650000e-01 -4.7064000e-03 -3.3210000e-03 /
CHEB / -3.6783000e-03 -4.5245000e-04 -3.2762000e-04 /
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tSPC(77)+O(+m)=CH2CH2CH2OOH+CO(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #194 (C4H7O3J(350))     deltaHrxn(T=298K) = -
92.85040516668515 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9485000e+00 -4.5420000e-03 -3.1601000e-03 /
CHEB / 5.8308000e+00 4.9490000e-03 3.4431000e-03 /
CHEB / 1.6516000e+00 3.6354000e-04 2.5320000e-04 /
CHEB / 4.4273000e-01 -6.4103000e-04 -4.4598000e-04 /
CHEB / 8.7025000e-02 -2.4650000e-04 -1.7152000e-04 /

C3H4O+CH2OOH(+m)=CH2CH2CH2OOH+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
19.9880045717688 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0769000e+01 -2.5759000e-04 -1.8036000e-04 /
CHEB / 1.8626000e+01 2.5762000e-04 1.8033000e-04 /
CHEB / 2.2923000e-01 6.2682000e-05 4.3993000e-05 /
CHEB / 2.4578000e-02 -4.0390000e-05 -2.8353000e-05 /
CHEB / -2.4237000e-02 -2.6037000e-05 -1.8251000e-05 /

C3H5OJ(12)+nSPC(102)(+m)=C3H4O-enone+CH2OOH(+m) 1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -44.95552669498089 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9339000e+00 -1.3890000e-02 -9.6964000e-03 /
CHEB / 1.8978000e+00 1.6166000e-02 1.1290000e-02 /
CHEB / 5.9356000e-01 -3.4734000e-05 -2.9720000e-05 /
CHEB / 1.1160000e-01 -2.1591000e-03 -1.5085000e-03 /
CHEB / -4.5133000e-02 -5.1987000e-04 -3.6124000e-04 /

iC4H7OJ(48)+O2(+m)=C3H4O-enone+CH2OOH(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) =
1.3900055211601483 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1734000e-01 -3.3635000e-01 -1.5955000e-01 /
CHEB / 7.3186000e+00 4.2993000e-01 1.9061000e-01 /
CHEB / 5.9687000e-01 -4.7134000e-02 -1.8597000e-04 /
CHEB / 9.7562000e-02 -5.7868000e-02 -3.2416000e-02 /
CHEB / -2.8117000e-02 -3.1618000e-03 -7.7487000e-03 /

C3H4O-enone+CH2OOH(+m)=C3H7O2+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
36.0061129476466 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4895000e+01 -1.3890000e-02 -9.6964000e-03 /
CHEB / 1.8195000e+01 1.6166000e-02 1.1290000e-02 /
CHEB / 8.4180000e-01 -3.4734000e-05 -2.9720000e-05 /
CHEB / 2.0644000e-01 -2.1591000e-03 -1.5085000e-03 /
CHEB / -2.1240000e-03 -5.1987000e-04 -3.6124000e-04 /
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tSPC(213)+H(+m)=C3H4O-enone+CH2OOH(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
5.308784803452291 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.3383000e-01 -2.8878000e-01 -9.4591000e-02 /
CHEB / 7.1831000e+00 3.8506000e-01 1.1118000e-01 /
CHEB / 1.0580000e+00 -6.3212000e-02 6.7850000e-03 /
CHEB / 2.0955000e-01 -5.2370000e-02 -2.7689000e-02 /
CHEB / -1.5099000e-02 9.3581000e-03 -2.8142000e-03 /

C3H4O-enone+CH2OOH(+m)=HO2+C4H6Oi-13(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
25.45740244459709 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0562000e+00 -2.1255000e-01 -9.3411000e-02 /
CHEB / 7.0788000e+00 2.6887000e-01 1.0581000e-01 /
CHEB / 6.4782000e-01 -1.9368000e-02 1.2653000e-02 /
CHEB / 9.4326000e-02 -4.6071000e-02 -2.5423000e-02 /
CHEB / -4.2517000e-02 -3.6336000e-03 -7.9053000e-03 /

HO2+tSPC(110)(+m)=C3H4O-enone+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
27.947196833383593 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9475000e+00 -4.7357000e-03 -3.0782000e-03 /
CHEB / 3.8767000e+00 4.9943000e-03 3.1693000e-03 /
CHEB / 1.0561000e+00 7.5162000e-04 5.9363000e-04 /
CHEB / 1.6073000e-01 -9.4754000e-04 -6.1385000e-04 /
CHEB / -4.1668000e-02 -2.0664000e-04 -1.7051000e-04 /

CH2OOH+C3H3OH(+m)=C3H4O-enone+CH2OOH(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
18.407955508028643 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.8230000e+00 -3.6150000e-01 -1.6102000e-01 /
CHEB / 7.3319000e+00 4.5648000e-01 1.8920000e-01 /
CHEB / 9.3052000e-01 -4.6202000e-02 2.3262000e-03 /
CHEB / 1.2753000e-01 -5.8300000e-02 -3.0890000e-02 /
CHEB / -1.5613000e-02 -4.1803000e-03 -7.7244000e-03 /

tSPC(77)+O(+m)=C3H4O-enone+CH2OOH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) = -
72.48238938468384 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.0980000e-01 -1.5947000e-03 -1.1137000e-03 /
CHEB / 3.7321000e+00 1.6213000e-03 1.1328000e-03 /
CHEB / 1.0269000e+00 2.6356000e-04 1.8378000e-04 /
CHEB / 2.6243000e-01 -1.8174000e-04 -1.2726000e-04 /
CHEB / 5.6622000e-02 -1.2810000e-04 -8.9415000e-05 /
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C3H4O+CH2OOH(+m)=C3H4O-enone+CH2OOH(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #194 (C4H7O3J(350))      deltaHrxn(T=298K) =
0.3800112102325013 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.7529000e+00 -5.0497000e-01 -2.2882000e-01 /
CHEB / 8.7483000e+00 6.7034000e-01 2.8729000e-01 /
CHEB / 9.2486000e-01 -1.1533000e-01 -2.3804000e-02 /
CHEB / 2.0417000e-01 -7.1653000e-02 -4.0683000e-02 /
CHEB / 7.3813000e-03 5.1773000e-03 -4.7462000e-03 /

C3H4O-enone+CH2OOH(+m)=CH2CH2CH2OOH+CO(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #194 (C4H7O3J(350))
      deltaHrxn(T=298K) = -20.368015782001304 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.7045000e+01 -2.2498000e-03 -1.5673000e-03 /
CHEB / 2.0863000e+01 2.1624000e-03 1.5064000e-03 /
CHEB / 9.9769000e-01 5.7269000e-04 3.9911000e-04 /
CHEB / 2.4895000e-01 -3.2053000e-04 -2.2348000e-04 /
CHEB / 2.0293000e-02 -2.1186000e-04 -1.4767000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     HOCHOOH     -25.83      77.47 18.14 20.12 21.93 23.68 26.4  28.62
      29.35 null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

aC3H4+HOCHOOH(+m)=O2+iC4H7OJ(15)(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O3J(368))  deltaHrxn(T=298K) = -
30.426769360975886 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.6211000e+00 -3.4938000e-01 -2.3560000e-01 /
CHEB / 2.6060000e+00 4.6769000e-01 2.6446000e-01 /
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CHEB / -3.7676000e-01 -3.9610000e-03 4.1833000e-02 /
CHEB / -1.7990000e-01 -1.1132000e-01 -4.4874000e-02 /
CHEB / -6.5745000e-02 -5.0989000e-02 -3.8859000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

iC4H5OJ(14)+O(+m)=sC3H5+CO2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #668 (spc11)      deltaHrxn(T=298K) = -95.59980257450889
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3525000e+01 -1.8936000e-05 -1.3181000e-05 /
CHEB / -4.0952000e-01 1.4164000e-05 9.8590000e-06 /
CHEB / 2.9467000e-03 3.9609000e-08 2.7589000e-08 /
CHEB / 2.1773000e-02 -2.9650000e-06 -2.0638000e-06 /
CHEB / 9.6319000e-03 -1.5492000e-06 -1.0784000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H5OJ      27.09 76.26 18.34 21.54 24.52 27.2  31.62 34.9  39.89
      null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     iC4H7OJ(17) -2.16 80.25 24.19 29.61 34.26 38.15 44.29 48.75 55.48
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:
```

```
iC4H7OJ(17)+O(+m)=C3H5OJ+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #813 (spc12)      deltaHrxn(T=298K) = -56.2441306188075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3312000e+01 -9.7027000e-04 -6.7491000e-04 /
CHEB / -2.4167000e-01 9.7907000e-04 6.8093000e-04 /
CHEB / 4.0213000e-03 9.6187000e-05 6.6979000e-05 /
CHEB / 1.3989000e-02 -1.4567000e-04 -1.0129000e-04 /
CHEB / 8.1752000e-03 -5.6227000e-05 -3.9139000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     C3H5OJ(12)        -1.58 70.39 18.06 21.84 25.19 28.08 32.66 36.06
      41.31 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OCH2CH2CH3  -9.17 75.06 20.0  24.84 29.16 32.91 38.84 43.25 48.01
      null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     iC4H7OJ(48) -2.2  83.37 23.03 28.2  33.04 36.99 43.43 48.09 53.71
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

CH2O+C3H5OJ(12)(+m)=OCH2CH2CH3+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #964 (spc13) deltaHrxn(T=298K) = -8.059311869863805
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8780000e+01 3.9657000e-06 2.7604000e-06 /
CHEB / 2.5913000e+01 6.7128000e-06 4.6725000e-06 /
CHEB / 1.4320000e-01 4.4244000e-06 3.0796000e-06 /
CHEB / 3.4054000e-04 2.2115000e-06 1.5393000e-06 /
CHEB / -4.4140000e-02 5.8611000e-07 4.0802000e-07 /

iC4H7OJ(48)+O(+m)=CH2O+C3H5OJ(12)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #964 (spc13) deltaHrxn(T=298K) = -84.87128355261949
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3301000e+01 4.6056000e-06 3.2057000e-06 /
CHEB / -4.5690000e-01 7.8464000e-06 5.4614000e-06 /
CHEB / -1.3596000e-01 5.0595000e-06 3.5217000e-06 /
CHEB / -1.0766000e-01 2.2141000e-06 1.5412000e-06 /
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CHEB / -9.1016000e-02 9.6136000e-08 6.7075000e-08 /

iC4H7OJ(48)+O(+m)=OCH2CH2CH3+CO(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #964 (spc13)      deltaHrxn(T=298K) = -92.93059542248331
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.1282000e+00 -1.0340000e-03 -7.1929000e-04 /
CHEB / 3.3780000e+00 8.2051000e-04 5.7073000e-04 /
CHEB / 1.1050000e+00 3.2420000e-04 2.2554000e-04 /
CHEB / 2.4022000e-01 -3.6236000e-05 -2.5142000e-05 /
CHEB / -1.6425000e-04 -5.7932000e-05 -4.0284000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H7-2            21.02 69.01 16.58 20.27 24.03 27.49 33.13 37.52
      44.42 null
!     CO2               -94.05      51.08 8.91  9.86  10.65 11.31 12.32
      12.99 13.93 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     iC4H7OJ(51) -14.3 80.77 22.74 28.03 33.0  37.03 43.54 48.2  52.91
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

iC4H7OJ(51)+O(+m)=C3H7-2+CO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1065 (spc14)     deltaHrxn(T=298K) = -118.2677134982669
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3309000e+01 5.1009000e-10 3.5506000e-10 /
CHEB / -2.4089000e-01 9.9293000e-10 6.9116000e-10 /
CHEB / 5.6558000e-06 9.1576000e-10 6.3744000e-10 /
CHEB / 1.3564000e-02 7.9901000e-10 5.5618000e-10 /
CHEB / 4.7870000e-03 6.5539000e-10 4.5620000e-10 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     C3H5OJ(17)  19.42 73.31 19.06 22.62 25.73 28.35 32.45 35.48 40.34
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

iC4H7OJ(15)+O(+m)=CH2O+C3H5OJ(17)(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1176 (spc15)      deltaHrxn(T=298K) = -
56.24413070422744 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.4020000e+01 -3.1011000e-08 -2.2183000e-08 /
CHEB / -8.2477000e-01 3.8044000e-08 2.7303000e-08 /
CHEB / 4.2097000e-03 6.6048000e-09 4.4335000e-09 /
CHEB / 1.4260000e-02 -6.5901000e-09 -4.7064000e-09 /
CHEB / 8.3411000e-03 -3.0013000e-09 -2.0403000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     acetone     -51.56      70.09 17.97 22.0  25.89 29.34 34.93 39.15
      44.77 null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     iC4H7OJ(30) -10.03      77.94 24.19 29.26 33.77 37.63 43.83 48.46
      55.63 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

iC4H7OJ(30)+O(+m)=acetone+HCO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1356 (spc16)     deltaHrxn(T=298K) = -90.67057366577741
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3908000e+01 3.9623000e-09 2.7580000e-09 /
CHEB / -7.9352000e-01 7.5993000e-09 5.2897000e-09 /
CHEB / -3.9142000e-02 6.8462000e-09 4.7655000e-09 /
CHEB / -2.0805000e-02 5.8465000e-09 4.0696000e-09 /
CHEB / -2.7350000e-02 4.7158000e-09 3.2826000e-09 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
```

```
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!Here are the path reactions and their high-P limit kinetics:
!     O2+H=HO2                8.1500000e+12      0.00000
7.6000000e+02
!     O+OH=HO2                1.0000000e+13      0.00000
0.0000000e+00

O+OH(+m)=HO2(+m)  1.0E0 0.0 0.0     !NetReaction from PDepNetwork #1
(HO2) High-P Limit: Oa_R_Recombination estimate: (Average:) Oa
O_pri_rad         deltaHrxn(T=298K) = -65.252881032273 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0042000e+01 1.9822000e+00 -1.2241000e-02 /
CHEB / -9.7309000e-01 1.7354000e-02 1.1883000e-02 /
CHEB / -3.5932000e-01 1.0709000e-03 7.7808000e-04 /
CHEB / -1.4521000e-01 -5.5927000e-04 -3.7879000e-04 /
CHEB / -6.3300000e-02 -3.7135000e-04 -2.5794000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     H2O2              -32.6 55.66 10.42 11.44 12.34 13.32 14.3  15.22
      16.86 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     HO2               0.43  54.74 8.43  8.76  9.27  10.02 10.75 11.56
      12.96 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:
!     OH+OH=H2O2              1.5700000e+13      0.00000
0.0000000e+00
!     HO2+H=H2O2              1.4157154e+13      -0.15000
2.9166667e+02

HO2+H(+m)=H2O2(+m)      1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#2 (H2O2) High-P Limit: R_Recombination estimate: (Average:) O_rad/NonDe
H_rad       deltaHrxn(T=298K) = -82.02126952571678 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.0437000e+00 2.0000000e+00 -2.2968000e-05 /
CHEB / -6.4444000e-01 2.4500000e-05 1.7054000e-05 /
```

```
CHEB / -2.8608000e-01 7.0262000e-06 4.8907000e-06 /
CHEB / -9.4911000e-02 4.4593000e-07 3.1044000e-07 /
CHEB / -3.5293000e-02 -6.4696000e-07 -4.5031000e-07 /

HO2+H(+m)=OH+OH(+m)     1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#2 (H2O2)   deltaHrxn(T=298K) = -30.787042275997763 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2843000e+01 -3.2701000e-05 -2.2762000e-05 /
CHEB / -1.0863000e-01 2.4799000e-05 1.7262000e-05 /
CHEB / 8.4777000e-04 6.9820000e-06 4.8600000e-06 /
CHEB / 3.9202000e-02 3.0491000e-07 2.1228000e-07 /
CHEB / 2.4302000e-02 -7.3507000e-07 -5.1165000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H7O-13          -2.41 80.44 22.13 27.78 32.68 36.83 43.32 48.0
      53.09 null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!Here are the path reactions and their high-P limit kinetics:

C4H7O-13+O(+m)=C3H4O+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (spc1)   deltaHrxn(T=298K) = -81.04188536185816 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3129000e+01 3.3697000e-06 2.3456000e-06 /
CHEB / -7.5896000e-01 -4.2946000e-07 -2.9892000e-07 /
CHEB / -2.5703000e-01 -1.8870000e-06 -1.3135000e-06 /
CHEB / -1.4377000e-01 -1.0726000e-06 -7.4665000e-07 /
CHEB / -7.7014000e-02 -2.0824000e-07 -1.4495000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H               134.46      51.51 10.05 10.42 10.71 10.96 11.47
      11.95 13.73 null
!     HCCOH             20.43 58.71 13.22 14.88 16.16 17.73 19.15 20.3
      22.02 null
```

```
!     C4H2              105.06      59.78 17.64 20.1  21.78 23.02 24.94
      26.38 28.84 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

C2H+HCCOH(+m)=C4H2+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #17 (spc2)  deltaHrxn(T=298K) = -40.50615582293431 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2931000e+01 -1.0013000e-04 -7.0571000e-05 /
CHEB / -1.8480000e-01 1.3914000e-04 9.8264000e-05 /
CHEB / -5.2506000e-04 -3.9376000e-05 -2.8142000e-05 /
CHEB / 1.7144000e-02 -1.0727000e-06 -5.2531000e-07 /
CHEB / 3.9244000e-03 9.4397000e-07 6.2826000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     HCCOH             20.43 58.71 13.22 14.88 16.16 17.73 19.15 20.3
      22.02 null
!     C4H4              68.17 65.12 17.41 21.68 24.25 27.71 31.23 33.72
      37.82 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

C2H3+HCCOH(+m)=C4H4+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #34 (spc3)  deltaHrxn(T=298K) = -14.558727525320142 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.7527000e+00 -1.2763000e-02 -8.7850000e-03 /
CHEB / 3.1746000e+00 1.6693000e-02 1.1468000e-02 /
CHEB / 3.1956000e-01 -3.1400000e-03 -2.1224000e-03 /
CHEB / 6.7034000e-02 -1.1539000e-03 -8.0986000e-04 /
CHEB / 1.7414000e-02 1.1162000e-04 7.3202000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H4              68.17 65.12 17.41 21.68 24.25 27.71 31.23 33.72
      37.82 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
```

```
!     CHCCHCHOH   26.04 72.81 21.36 26.28 29.2  32.79 36.28 38.62 42.53
      null
!     H                49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C3H2             120.52      62.42 13.2  15.02 16.44 17.7  19.48
      20.84 24.88 null
!     CH2OH            -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     C2H              134.46      51.51 10.05 10.42 10.71 10.96 11.47
      11.95 13.73 null
!     C2H4O            -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!Here are the path reactions and their high-P limit kinetics:

C3H2+CH2OH(+m)=C4H4+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (spc4)  deltaHrxn(T=298K) = -39.436177803280025 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3409000e+01 -5.0024000e-03 -4.2161000e-03 /
CHEB / -7.3420000e-01 6.9369000e-03 5.8570000e-03 /
CHEB / -8.9595000e-02 -1.6499000e-03 -1.4181000e-03 /
CHEB / -4.6506000e-02 -5.2609000e-04 -4.4458000e-04 /
CHEB / -3.6864000e-02 2.3072000e-04 2.1227000e-04 /

CHCCHCHOH+H(+m)=C3H2+CH2OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (spc4)  deltaHrxn(T=298K) = 41.88616518791621 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3152000e-01 -3.2797000e-02 -2.1725000e-02 /
CHEB / 1.2996000e+01 2.5284000e-02 1.4774000e-02 /
CHEB / -8.7095000e-02 1.9882000e-02 1.3591000e-02 /
CHEB / -2.1617000e-02 -3.7149000e-03 4.7056000e-04 /
CHEB / -8.5942000e-03 -9.4033000e-03 -5.7679000e-03 /

C2H+C2H4O(+m)=C4H4+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (spc4)  deltaHrxn(T=298K) = -27.357328543262675 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2701000e+01 -9.2507000e-01 -2.7185000e-01 /
CHEB / -1.0936000e-01 9.7016000e-01 2.2560000e-01 /
CHEB / -7.4735000e-02 1.1075000e-01 9.4702000e-02 /
CHEB / -1.4275000e-01 -9.5705000e-02 -5.0815000e-03 /
CHEB / -7.5712000e-02 -6.1632000e-02 -2.9926000e-02 /

CHCCHCHOH+H(+m)=C2H+C2H4O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (spc4)  deltaHrxn(T=298K) = 29.807315927898873 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2534000e+00 -8.1436000e-01 -2.1753000e-01 /
CHEB / 8.3837000e+00 8.2539000e-01 1.5124000e-01 /
CHEB / -3.4699000e-01 1.3761000e-01 1.0979000e-01 /
CHEB / -1.7498000e-01 -7.5804000e-02 7.9072000e-03 /
CHEB / -6.3843000e-02 -6.7093000e-02 -3.1842000e-02 /

C2H+C2H4O(+m)=C3H2+CH2OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #85 (spc4)  deltaHrxn(T=298K) = 12.078849260017344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 6.8620000e+00 -4.1481000e-01 -2.0671000e-01 /
CHEB / 4.8955000e+00 4.8296000e-01 2.2683000e-01 /
CHEB / 1.8771000e-01 -1.5307000e-03 1.6864000e-02 /
CHEB / -4.5674000e-03 -6.2992000e-02 -2.9204000e-02 /
CHEB / -2.4147000e-02 -1.5430000e-02 -1.3161000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C2H4O             -29.61      62.91 14.15 17.32 19.97 22.08 25.19
      27.44 31.09 null
!     C2H3O-1           29.49 64.3  13.96 16.57 18.61 20.16 22.37 23.95
      26.56 null
!     CH2CHCHCHOH -16.05      75.67 23.07 28.9  33.47 36.92 41.89 45.42
      51.05 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

CH2CHCHCHOH+OH(+m)=C2H4O+C2H3O-1(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #155 (spc6)  deltaHrxn(T=298K) = 6.609649754764309
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.2095000e+00 -1.7971000e-01 -1.0806000e-01 /
CHEB / 6.7632000e+00 2.2962000e-01 1.3380000e-01 /
CHEB / 2.2120000e-01 -2.7944000e-02 -9.5879000e-03 /
CHEB / 3.3962000e-02 -2.7698000e-02 -1.8556000e-02 /
CHEB / -1.1835000e-02 1.4486000e-04 -1.8123000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     iC4H7OJ(30) -10.03      77.94 24.19 29.26 33.77 37.63 43.83 48.46
      55.63 null
!     iC4H7OJ(48) -2.2  83.37 23.03 28.2  33.04 36.99 43.43 48.09 53.71
      null
!     iC4H7OJ(51) -14.3 80.77 22.74 28.03 33.0  37.03 43.54 48.2  52.91
      null
!     iC4H7OJ(17) -2.16 80.25 24.19 29.61 34.26 38.15 44.29 48.75 55.48
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     C3H3OH      4.59  68.91 18.05 21.72 24.67 27.08 30.49 32.94 36.79
      null
```

```
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
!     HCC[CH3]2   55.3  72.75 21.39 25.9  29.94 33.42 39.09 43.4  50.18
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     CH2O              -25.95      52.3  8.47  9.38  10.46 11.52 13.37
      14.81 14.81 null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!Here are the path reactions and their high-P limit kinetics:
!     C3H3OH+CH3=iC4H7OJ(15)  1.5800000e+11      0.00000
4.9700000e+03
!     C4H6Oi-13+H=iC4H7OJ(15) 2.3501400e+11      0.30815
4.9629937e+03
!     tSPC(110)+H=iC4H7OJ(15) 1.4157154e+13      -0.15000
2.9166667e+02
!     iC4H7OJ(30)=iC4H7OJ(15) 1.4106558e+11      0.61833
2.7168333e+04
!     C4H6Oi-12+H=iC4H7OJ(30) 5.2263889e+12      0.04600
5.0666667e+03
!     C4H6Oi-13+H=iC4H7OJ(30) 2.1300000e+13      0.00000
5.0000000e+02
!     tSPC(110)+H=iC4H7OJ(30) 5.0000000e+13      0.00000
0.0000000e+00
!     iC4H7OJ(48)=iC4H7OJ(30) 6.2339791e+09      0.93630
3.7689907e+04
!     iC4H7OJ(30)=iC4H7OJ(51) 2.0320555e+08      1.13906
3.4790987e+04
!     HCC[CH3]2+O=iC4H7OJ(30) 1.0000000e+13      0.00000
0.0000000e+00
!     iC4H7OJ(17)=iC4H7OJ(15) 2.1620731e+09      0.93000
3.2050000e+04
!     C4H7OJ(79)=iC4H7OJ(15)  8.1282219e+08      1.13906
3.4790987e+04
!     CH2O+sC3H5=C4H7OJ(79)   3.2847733e+07      1.50370
7.3354000e+03
!     C4H6Oi-13+H=C4H7OJ(79)  1.0000000e+11      0.00000
1.1900000e+04
!     tSPC(110)+H=C4H7OJ(79)  1.4157154e+13      -0.15000
2.9166667e+02
!     C4H7OJ(79)=iC4H7OJ(17)  9.0000000e+11      0.00000
2.9400000e+04
!     O+iC4H7=C4H7OJ(79)      1.0000000e+13      0.00000
0.0000000e+00
```

```
CH2O+sC3H5(+m)=iC4H7OJ(30)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #7 (iC4H7OJ(15))  deltaHrxn(T=298K) = -45.62538127876018
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1668000e+00 1.3192000e+00 -5.1992000e-01 /
CHEB / 1.2894000e+00 2.6067000e+00 1.0696000e-02 /
CHEB / -2.4479000e+00 8.2574000e-01 5.3613000e-02 /
CHEB / -1.5295000e+00 8.9592000e-02 8.2767000e-02 /
CHEB / -8.1918000e-01 -1.3891000e-01 3.1447000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-i1    -38.26      82.01 24.81 30.17 35.04 39.27 46.13 51.21
      58.97 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     CH2OH             -3.59 58.19 10.74 12.52 13.96 15.19 17.1  18.53
      20.8  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H8O-i2    -45.93      79.05 25.53 31.25 36.25 40.42 46.96 51.79
      59.42 null
!Here are the path reactions and their high-P limit kinetics:

iC4H5OJ(14)+CH2OH(+m)=C4H8O-i1+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #137 (C5H8O2JJ(381))     deltaHrxn(T=298K) = -
64.64332743401413 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0794000e+00 1.2073000e-15 -5.7957000e-16 /
CHEB / 2.8126000e+00 -1.1323000e-15 1.8417000e-15 /
CHEB / 3.6448000e-02 2.1005000e-15 -9.5822000e-16 /
CHEB / 1.8896000e-02 -7.3928000e-16 1.3756000e-15 /
CHEB / -4.4112000e-03 1.3593000e-15 -5.2168000e-16 /

C4H8O-i1+CO(+m)=C4H8O-i2+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #137 (C5H8O2JJ(381))    deltaHrxn(T=298K) = -
7.669293951907498 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.4796000e+01 -1.2774000e-16 9.7099000e-16 /
CHEB / 3.0190000e+01 2.6441000e-15 -5.5779000e-16 /
CHEB / 3.3784000e-01 -1.7022000e-15 3.0412000e-15 /
```

```
CHEB / 1.1218000e-01 4.6680000e-15 -2.5374000e-15 /
CHEB / 2.9339000e-02 -3.9761000e-15 4.6014000e-15 /

iC4H5OJ(14)+CH2OH(+m)=C4H8O-i2+CO(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #137 (C5H8O2JJ(381))     deltaHrxn(T=298K) = -
72.31262138592163 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3203000e+01 -7.5199000e-12 -5.2343000e-12 /
CHEB / 2.7093000e+01 -1.4732000e-11 -1.0256000e-11 /
CHEB / 7.9209000e-01 -1.3832000e-11 -9.6253000e-12 /
CHEB / 2.3438000e-01 -1.2379000e-11 -8.6226000e-12 /
CHEB / 5.6696000e-02 -1.0471000e-11 -7.2811000e-12 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8O-i2    -45.93      79.05 25.53 31.25 36.25 40.42 46.96 51.79
      59.42 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     OH                9.32  43.91 7.16  7.09  7.06  7.06  7.15  7.33
      7.88  null
!     C4H8O-i3    -51.2 79.65 23.57 29.46 34.96 39.45 46.7  51.93 57.55
      null
!     O                 59.55 38.49 5.23  5.14  5.09  5.06  5.02  5.0
      4.98  null
!     C3H7-2            21.02 69.01 16.58 20.27 24.03 27.49 33.13 37.52
      44.42 null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!Here are the path reactions and their high-P limit kinetics:

C4H8O-i2+CO(+m)=C4H8O-i3+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #212 (C5H8O2JJ(408))    deltaHrxn(T=298K) = -
5.269267092314344 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.1473000e+01 2.4525000e-16 3.6720000e-16 /
CHEB / 3.6081000e+01 1.3584000e-15 -2.9386000e-17 /
CHEB / 4.0198000e-01 -1.4165000e-15 2.2666000e-15 /
CHEB / 1.6702000e-01 4.2528000e-15 -2.6639000e-15 /
CHEB / 6.6661000e-02 -4.5136000e-15 4.6545000e-15 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H6Oi-12   -21.8 75.1  22.2  26.42 30.33 34.8  39.5  43.82 50.51
      null
```

```
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     iC4H5OJ(14) 3.56  73.25 22.95 27.49 31.07 33.96 38.52 41.67 45.78
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!Here are the path reactions and their high-P limit kinetics:

C4H6Oi-12+CO(+m)=C4H6Oi-13+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #341 (C5H6O2JJ(577))    deltaHrxn(T=298K) = -
5.535613182213975 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5993000e+01 1.0516000e-13 7.4288000e-14 /
CHEB / 3.1443000e+01 2.0967000e-13 1.4283000e-13 /
CHEB / 3.8542000e-01 1.9268000e-13 1.3864000e-13 /
CHEB / 1.3404000e-01 1.8043000e-13 1.1881000e-13 /
CHEB / 4.2488000e-02 1.4452000e-13 1.0863000e-13 /

iC4H5OJ(14)+HCO(+m)=C4H6Oi-12+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #341 (C5H6O2JJ(577))     deltaHrxn(T=298K) = -
62.17740669819822 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5809000e+01 -5.9960000e-12 -4.1722000e-12 /
CHEB / 2.9749000e+01 -1.1748000e-11 -8.1804000e-12 /
CHEB / 5.3867000e-01 -1.1044000e-11 -7.6830000e-12 /
CHEB / 2.0274000e-01 -9.8972000e-12 -6.8949000e-12 /
CHEB / 7.5478000e-02 -8.3885000e-12 -5.8318000e-12 /

iC4H5OJ(14)+HCO(+m)=C4H6Oi-13+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #341 (C5H6O2JJ(577))     deltaHrxn(T=298K) = -
67.71301988041219 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3891000e+00 1.2260000e-15 -7.3852000e-16 /
CHEB / 2.0937000e+00 -1.5124000e-15 1.8835000e-15 /
CHEB / -1.3358000e-01 2.1734000e-15 -1.2866000e-15 /
CHEB / 5.7256000e-02 -1.1272000e-15 1.4648000e-15 /
CHEB / 2.4629000e-02 1.4901000e-15 -8.3705000e-16 /

tSPC(110)+CO(+m)=C4H6Oi-12+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #341 (C5H6O2JJ(577))    deltaHrxn(T=298K) = -
47.868986095766715 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.9316000e+01 1.0611000e-13 7.3477000e-14 /
```

```
CHEB / 3.2551000e+01 2.0788000e-13 1.4435000e-13 /
CHEB / 2.5759000e-01 1.9415000e-13 1.3740000e-13 /
CHEB / 9.4285000e-02 1.7941000e-13 1.1967000e-13 /
CHEB / 3.0541000e-02 1.4508000e-13 1.0815000e-13 /

tSPC(110)+CO(+m)=C4H6Oi-13+CO(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #341 (C5H6O2JJ(577))    deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.2631000e+00 -1.2050000e-15 -2.4194000e-15 /
CHEB / 3.9706000e+00 -6.0280000e-15 -8.4176000e-16 /
CHEB / -7.8543000e-01 -7.2303000e-16 -2.8966000e-15 /
CHEB / -8.1668000e-02 -1.5719000e-15 1.0223000e-15 /
CHEB / 3.1603000e-02 2.2201000e-15 7.0097000e-16 /

iC4H5OJ(14)+HCO(+m)=tSPC(110)+CO(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #341 (C5H6O2JJ(577))     deltaHrxn(T=298K) = -
14.308420602431505 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3306000e+01 5.5327000e-16 -4.7064000e-16 /
CHEB / 1.9757000e+01 -6.2539000e-16 5.7493000e-16 /
CHEB / -1.3893000e-01 -4.6327000e-16 5.4943000e-16 /
CHEB / 5.5383000e-02 2.2479000e-15 -1.6173000e-15 /
CHEB / 2.3891000e-02 -3.1082000e-15 3.0504000e-15 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(213)   -45.6 92.58 31.18 37.39 42.35 46.37 52.4  56.68 61.44
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     C3H5OJ(17)  22.25 72.17 19.21 23.32 26.93 29.77 33.8  36.58 40.96
!MRH CBS-QB3 w/1DHR corrections
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     iC4H7OJ(15) -9.83 77.3  24.91 30.69 35.47 39.3  45.12 49.33 55.93
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
```

```
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C3H5OJ(17)+nSPC(102)(+m)=tSPC(213)+H(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H7O3J(344))  deltaHrxn(T=298K) = -
66.85389144475766 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8564000e+00 -5.8241000e-04 -4.0552000e-04 /
CHEB / 1.9089000e+00 5.4788000e-04 3.8147000e-04 /
CHEB / 7.0253000e-01 1.3697000e-04 9.5383000e-05 /
CHEB / 1.8889000e-01 -4.6726000e-05 -3.2535000e-05 /
CHEB / 1.9361000e-02 -5.0286000e-05 -3.5018000e-05 /

C3H5OJ(17)+nSPC(102)(+m)=HO2+C4H6Oi-13(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H7O3J(344)) deltaHrxn(T=298K)
= -97.62007869280706 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3068000e+00 -1.9005000e-04 -1.3239000e-04 /
CHEB / 3.5932000e-01 2.4489000e-04 1.7057000e-04 /
CHEB / 2.1705000e-01 1.8669000e-05 1.3015000e-05 /
CHEB / 1.1291000e-02 -4.6318000e-05 -3.2256000e-05 /
CHEB / -4.6923000e-02 -2.8685000e-05 -1.9978000e-05 /

C3H5OJ(17)+nSPC(102)(+m)=HO2+tSPC(110)(+m)      1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H7O3J(344)) deltaHrxn(T=298K)
= -44.21547941482636 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.8013000e+00 -1.2725000e-03 -8.8552000e-04 /
CHEB / 1.8078000e+00 1.1695000e-03 8.1377000e-04 /
CHEB / 8.0998000e-01 2.9376000e-04 2.0450000e-04 /
CHEB / 2.1932000e-01 -9.3595000e-05 -6.5107000e-05 /
CHEB / 1.6433000e-02 -9.3214000e-05 -6.4880000e-05 /

tSPC(213)+H(+m)=iC4H7OJ(15)+O2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H7O3J(344)) deltaHrxn(T=298K) = -15.647727332490781
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.9961000e+00 -4.5004000e-02 -3.3295000e-02 /
CHEB / 2.8383000e+00 6.2000000e-02 4.5845000e-02 /
CHEB / 5.2688000e-01 -1.5021000e-02 -1.0890000e-02 /
CHEB / 8.0760000e-02 -4.1786000e-03 -3.4811000e-03 /
CHEB / -4.3767000e-02 1.4266000e-03 1.2331000e-03 /

iC4H7OJ(15)+O2(+m)=HO2+C4H6Oi-13(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H7O3J(344))  deltaHrxn(T=298K) = -
15.1184599155586 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.7581000e+00 -8.2445000e-02 -5.8742000e-02 /
CHEB / 5.2620000e+00 1.1655000e-01 8.1888000e-02 /
CHEB / 1.0064000e-01 -2.9546000e-02 -1.8842000e-02 /
CHEB / -5.2585000e-02 -1.1349000e-02 -8.9913000e-03 /
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CHEB / -7.4545000e-02 5.2324000e-03 3.1331000e-03 /

HO2+tSPC(110)(+m)=iC4H7OJ(15)+O2(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H7O3J(344))  deltaHrxn(T=298K) = -
38.286139362422084 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.2064000e+00 -1.2795000e-03 -8.9321000e-04 /
CHEB / 1.7357000e+00 1.0784000e-03 7.5430000e-04 /
CHEB / 4.0384000e-01 4.4734000e-04 3.1031000e-04 /
CHEB / 2.9295000e-02 -7.8821000e-05 -5.5021000e-05 /
CHEB / -5.9466000e-02 -1.3097000e-04 -9.0963000e-05 /

C3H5OJ(17)+nSPC(102)(+m)=iC4H7OJ(15)+O2(+m)     1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (C4H7O3J(344)) deltaHrxn(T=298K)
= -82.50161877724844 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3861000e+01 1.1724000e-06 8.1603000e-07 /
CHEB / -1.0603000e+00 1.6906000e-06 1.1769000e-06 /
CHEB / -5.7910000e-02 4.5693000e-07 3.1806000e-07 /
CHEB / -2.5403000e-02 -2.0844000e-07 -1.4510000e-07 /
CHEB / -1.8382000e-02 -3.8455000e-07 -2.6768000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     CO                -26.42      47.21 6.97  7.0   7.14  7.28  7.62
      7.93  6.22  null
!     CH2               92.34 46.3  8.16  8.76  9.0   9.18  9.82  10.51
      11.16 null
!     C3H3O-enone 10.58 66.0  16.82 20.07 22.49 24.41 27.35 29.39 31.57
      null
!     HCO               10.4  53.67 8.28  8.73  9.27  9.79  10.74 11.49
      10.39 null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!Here are the path reactions and their high-P limit kinetics:

C3H3O-enone+HCO(+m)=C3H4O+CO(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #5 (C4H4O2JJ(378))      deltaHrxn(T=298K) = -
67.71302000976182 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7097000e+00 -2.4680000e-08 -1.7179000e-08 /
CHEB / 1.7187000e+00 -4.8402000e-08 -3.3692000e-08 /
CHEB / 2.8763000e-02 -4.5571000e-08 -3.1721000e-08 /
CHEB / 5.0268000e-02 -4.0981000e-08 -2.8526000e-08 /
CHEB / 3.4751000e-02 -3.4819000e-08 -2.4237000e-08 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
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!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               34.81 46.37 9.14  10.18 10.81 11.34 12.57 13.71
      15.2  null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     aC3H5             40.75 62.05 14.83 18.67 21.94 24.67 28.9  32.03
      36.9  null
!     CH2CHCH2O   22.15 72.99 17.7  21.45 24.85 27.83 32.58 36.01 41.06
      null
!     H                 49.0  2.61  -0.77 -1.36 -1.91 -2.4  -3.16 -3.74
      -4.66 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C2H3              71.62 56.61 10.01 11.97 13.66 15.08 17.32 19.05
      21.85 null
!     C3H4O             -20.32      67.39 17.01 20.92 24.08 26.62 30.56
      33.28 36.18 null
!     iC4H7       32.3  69.61 20.96 26.09 30.52 34.22 40.07 44.43 51.22
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     sC3H5             61.55 65.62 15.11 18.02 20.78 23.27 27.4  30.58
      35.63 null
!Here are the path reactions and their high-P limit kinetics:

tSPC(110)+aC3H5(+m)=C4H6Oi-13+aC3H5(+m)   1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #35 (C7H11OJ(540)) deltaHrxn(T=298K) = -
53.40459927798069 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2923000e+01 4.2038000e-10 2.9261000e-10 /
CHEB / -2.2588000e-01 2.0921000e-09 1.4562000e-09 /
CHEB / -2.1535000e-02 1.9623000e-09 1.3659000e-09 /
CHEB / -1.3007000e-04 1.3873000e-09 9.6564000e-10 /
CHEB / -2.3666000e-03 9.6215000e-10 6.6972000e-10 /

C4H6Oi-13+aC3H5(+m)=C3H4O+iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (C7H11OJ(540))      deltaHrxn(T=298K) = -
1.4298603128526963 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.5791000e+00 -1.0659000e-09 -7.4424000e-10 /
CHEB / 1.1264000e+01 2.0112000e-09 1.4036000e-09 /
CHEB / 3.9175000e-01 1.4818000e-09 1.0300000e-09 /
CHEB / 1.5768000e-01 4.7227000e-10 3.2864000e-10 /
CHEB / 6.8234000e-02 8.1470000e-11 5.7123000e-11 /

tSPC(110)+aC3H5(+m)=C3H4O+iC4H7(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #35 (C7H11OJ(540))      deltaHrxn(T=298K) = -
54.834459590833376 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8516000e+00 -6.1774000e-06 -4.3000000e-06 /
CHEB / 2.9156000e+00 4.5594000e-06 3.1737000e-06 /
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CHEB / 9.2111000e-01 2.2122000e-06 1.5398000e-06 /
CHEB / 2.7784000e-01 -2.4225000e-07 -1.6862000e-07 /
CHEB / 7.0191000e-02 -4.8612000e-07 -3.3837000e-07 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     nSPC(102)         51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57
      23.05 null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     CH2               93.85 46.59 8.3   8.66  8.98  9.28  9.87  10.47
      11.69
!     O           59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96  4.96
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     sSPC(2810)        -29.51      59.94 9.81  11.32 12.68 13.78 15.39
      16.47 17.98
!Here are the path reactions and their high-P limit kinetics:
!     O2+CH2=nSPC(102)        2.000e+13    0.00        0.00
!     O+CH2O=nSPC(102)        2.3501400e+11      0.30815
4.9629937e+03
!     O+CH2OJJ(70)=nSPC(102)  1.0000000e+13      0.00000
0.0000000e+00

O2+CH2(+m)=nSPC(102)(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nSPC(102)) High-P Limit: ReactionLibrary: MRH
      deltaHrxn(T=298K) = -43.415306461132026 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.9295000e+00 2.0013000e+00 8.7338000e-04 /
CHEB / 3.2162000e+00 2.4031000e-03 1.6723000e-03 /
CHEB / -5.7554000e-01 2.1093000e-03 1.4678000e-03 /
CHEB / -2.4488000e-01 1.6980000e-03 1.1815000e-03 /
CHEB / -1.0152000e-01 1.2527000e-03 8.7158000e-04 /

nSPC(102)(+m)=O+CH2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nSPC(102))    deltaHrxn(T=298K) = -17.688272187158713
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.0209000e+00 2.0000000e+00 -1.0571000e-05 /
CHEB / 1.7436000e+00 -2.8805000e-05 -2.0045000e-05 /
CHEB / -7.3678000e-01 -2.4569000e-05 -1.7096000e-05 /
CHEB / -3.3489000e-01 -1.8888000e-05 -1.3143000e-05 /
CHEB / -1.4416000e-01 -1.3117000e-05 -9.1263000e-06 /

O2+CH2(+m)=O+CH2O(+m)   1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#1 (nSPC(102))    deltaHrxn(T=298K) = -61.103578648290735 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3405000e+01 5.3459000e-08 3.7211000e-08 /
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CHEB / -5.6441000e-02 1.0384000e-07 7.2282000e-08 /
CHEB / 3.9539000e-03 9.5112000e-08 6.6205000e-08 /
CHEB / 2.8734000e-02 8.2041000e-08 5.7107000e-08 /
CHEB / 1.5011000e-02 6.6314000e-08 4.6160000e-08 /

nSPC(102)(+m)=sSPC(2810)+H(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nSPC(102))    deltaHrxn(T=298K) = -28.517350283179773
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3446000e+00 1.9999000e+00 -6.0658000e-05 /
CHEB / 6.9849000e+00 5.0571000e-04 3.5267000e-04 /
CHEB / -5.4389000e-01 -9.0256000e-05 -6.3162000e-05 /
CHEB / -2.7704000e-01 -7.6170000e-05 -5.2990000e-05 /
CHEB / -1.2816000e-01 -3.7732000e-05 -2.6170000e-05 /

O2+CH2(+m)=sSPC(2810)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nSPC(102))    deltaHrxn(T=298K) = -71.9326567443118
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5316000e+00 1.4222000e-06 9.7107000e-07 /
CHEB / 5.1071000e+00 1.4380000e-05 1.0033000e-05 /
CHEB / 1.1039000e-01 2.2585000e-07 1.5532000e-07 /
CHEB / 3.3427000e-02 -3.5486000e-06 -2.4726000e-06 /
CHEB / 1.7705000e-03 -1.9727000e-06 -1.3736000e-06 /

O+CH2O(+m)=sSPC(2810)+H(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (nSPC(102))    deltaHrxn(T=298K) = -10.829078096021064
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.8902000e+00 -1.4415000e-01 -1.2864000e-01 /
CHEB / 1.2022000e+00 1.3919000e-01 1.2549000e-01 /
CHEB / 3.2402000e-03 3.2036000e-02 2.4987000e-02 /
CHEB / -4.2435000e-02 -1.5787000e-02 -1.2947000e-02 /
CHEB / -2.7968000e-02 -1.2013000e-02 -9.1123000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     isoC3H7OH(1)      -64.83      74.2  21.77 26.89 31.47 35.35 41.49
      46.13 53.57
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H5O-2           -12.92      68.09 15.82 18.76 21.49 23.84 27.55
      30.36 34.89
!     CH3CH[OH]CH2      -14.14      76.56 22.67 26.97 30.74 33.91 38.93
      42.77 49.05
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
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!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH3C[OH]CH3       -22.33      74.56 21.77 26.05 29.95 33.3  38.64
      42.68 49.13
!     C3H7OJ(65)        -9.85 72.53 20.83 25.56 29.74 33.3  38.96 43.24
      50.0
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!Here are the path reactions and their high-P limit kinetics:
!     CH3+C2H5O-2=isoC3H7OH(1)      6.8000000e+14      -0.68000
0.0000000e+00
!     CH3CH[OH]CH2+H=isoC3H7OH(1)   1.0000000e+14      0.00000
0.0000000e+00
!     C3H7-2+OH=isoC3H7OH(1)        1.4157154e+13      -0.15000
2.9166667e+02
!     CH3C[OH]CH3+H=isoC3H7OH(1)    5.0000000e+13      0.00000
0.0000000e+00
!     C3H7OJ(65)+H=isoC3H7OH(1)     1.4157154e+13      -0.15000
2.9166667e+02
!     C3H6+H2O=isoC3H7OH(1)         6.5200000e+01      2.92000
5.0700000e+04

CH3CH[OH]CH2+H(+m)=CH3+C2H5O-2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -15.62807320010193
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3207000e+01 -1.0578000e+00 -1.5479000e-01 /
CHEB / 7.3391000e-01 9.3587000e-01 5.7612000e-02 /
CHEB / 2.1233000e-01 2.8019000e-01 9.3889000e-02 /
CHEB / -3.4179000e-02 -4.1443000e-02 4.2644000e-02 /
CHEB / -4.7836000e-02 -8.7555000e-02 -1.0537000e-02 /

C3H7-2+OH(+m)=CH3+C2H5O-2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -12.369021535748935
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1759000e+01 -1.1252000e+00 -1.3170000e-01 /
CHEB / 7.9370000e-01 9.8358000e-01 2.5942000e-02 /
CHEB / 1.9985000e-01 3.0480000e-01 9.3893000e-02 /
CHEB / -7.9568000e-02 -3.5697000e-02 4.9899000e-02 /
CHEB / -7.7724000e-02 -9.2678000e-02 -6.4475000e-03 /

CH3CH[OH]CH2+H(+m)=C3H7-2+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -3.259051664352995
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.5102000e+00 -9.3670000e-01 -1.7217000e-01 /
CHEB / 2.3157000e+00 9.0079000e-01 9.3328000e-02 /
CHEB / 5.3104000e-01 1.8887000e-01 9.8811000e-02 /
CHEB / 4.0823000e-02 -6.8774000e-02 2.0867000e-02 /
CHEB / -1.3567000e-02 -7.6406000e-02 -2.1636000e-02 /
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CH3C[OH]CH3+H(+m)=CH3+C2H5O-2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -7.439019048248376
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2484000e+01 -1.2611000e+00 -8.4310000e-02 /
CHEB / 1.2042000e+00 1.0418000e+00 -3.1933000e-02 /
CHEB / 2.9174000e-01 3.8373000e-01 7.8960000e-02 /
CHEB / -9.5002000e-02 -6.7734000e-03 6.5459000e-02 /
CHEB / -8.2341000e-02 -1.0315000e-01 8.6140000e-03 /

CH3CH[OH]CH2+H(+m)=CH3C[OH]CH3+H(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (isoC3H7OH)     deltaHrxn(T=298K) = -
8.189054151853554 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.7918000e+00 -1.0130000e+00 -1.5956000e-01 /
CHEB / 2.3049000e+00 9.3359000e-01 6.9333000e-02 /
CHEB / 6.2547000e-01 2.4034000e-01 9.7711000e-02 /
CHEB / 9.1469000e-02 -5.8461000e-02 3.4068000e-02 /
CHEB / 2.4085000e-03 -8.4452000e-02 -1.6555000e-02 /

CH3C[OH]CH3+H(+m)=C3H7-2+OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = 4.930002487500559
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 8.0308000e+00 -1.0746000e+00 -1.3968000e-01 /
CHEB / 3.6729000e+00 9.8089000e-01 4.0279000e-02 /
CHEB / 4.1620000e-01 2.6053000e-01 1.0017000e-01 /
CHEB / -9.2887000e-03 -5.5104000e-02 4.0772000e-02 /
CHEB / -3.9998000e-02 -8.9568000e-02 -1.3666000e-02 /

CH3+C2H5O-2(+m)=C3H6+H2O(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -74.54221695839459
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1091000e+01 -1.4316000e+00 -5.5143000e-02 /
CHEB / 1.0192000e+00 9.4136000e-01 -6.0815000e-02 /
CHEB / 2.3309000e-01 5.1903000e-01 2.3190000e-02 /
CHEB / -1.3280000e-01 1.4051000e-01 6.1093000e-02 /
CHEB / -1.3625000e-01 -5.4925000e-02 4.2067000e-02 /

CH3CH[OH]CH2+H(+m)=C3H6+H2O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -90.17029015849653
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2275000e+01 -1.1374000e+00 -1.5182000e-01 /
CHEB / 1.0410000e+00 9.0969000e-01 3.7730000e-02 /
CHEB / 1.5908000e-01 3.4923000e-01 8.3351000e-02 /
CHEB / -4.2437000e-02 1.1592000e-02 5.5931000e-02 /
CHEB / -5.2119000e-02 -7.7663000e-02 5.0176000e-03 /
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C3H7-2+OH(+m)=C3H6+H2O(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -86.91123849414353
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0940000e+01 -1.2113000e+00 -1.2536000e-01 /
CHEB / 1.0142000e+00 9.5133000e-01 4.4802000e-03 /
CHEB / 1.3792000e-01 3.7853000e-01 7.8571000e-02 /
CHEB / -8.5437000e-02 2.4830000e-02 6.1987000e-02 /
CHEB / -8.2716000e-02 -7.9506000e-02 1.1093000e-02 /

CH3C[OH]CH3+H(+m)=C3H6+H2O(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (isoC3H7OH)    deltaHrxn(T=298K) = -81.98123600664297
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2074000e+01 -1.3578000e+00 -7.3297000e-02 /
CHEB / 1.0728000e+00 9.8220000e-01 -5.0659000e-02 /
CHEB / 2.2619000e-01 4.6338000e-01 5.1018000e-02 /
CHEB / -8.6477000e-02 7.8890000e-02 6.8650000e-02 /
CHEB / -9.2076000e-02 -7.5732000e-02 2.9830000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C2H4              13.55 52.25 10.17 12.51 14.73 16.67 19.8  22.2
      26.08
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C2H5O-3           -2.66 66.84 15.8  18.82 21.65 24.13 28.15 31.21
      36.01
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

CH3+nSPC(102)(+m)=C2H5+O2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -56.24383782924884 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3451000e+01 -9.5683000e-07 -6.6672000e-07 /
CHEB / -1.1767000e+00 -8.5131000e-07 -5.9281000e-07 /
CHEB / -2.5500000e-01 4.9106000e-07 3.4247000e-07 /
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CHEB / -9.7472000e-02 8.5698000e-07 5.9706000e-07 /
CHEB / -5.4996000e-02 5.2338000e-07 3.6438000e-07 /

CH3+nSPC(102)(+m)=C2H4+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -69.73233975610651 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2043000e+01 1.0652000e-04 7.4238000e-05 /
CHEB / 1.5804000e-01 -9.6305000e-05 -6.7126000e-05 /
CHEB / 8.9765000e-02 -2.2096000e-05 -1.5403000e-05 /
CHEB / 1.8074000e-02 3.7597000e-06 2.6316000e-06 /
CHEB / -9.6096000e-03 6.1002000e-06 4.2556000e-06 /

C2H5+O2(+m)=C2H4+HO2(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -13.48850192685768 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1231000e+01 -6.6806000e-01 -1.9647000e-01 /
CHEB / 1.0106000e+00 7.2665000e-01 1.9091000e-01 /
CHEB / 4.7462000e-02 7.3556000e-02 4.3732000e-02 /
CHEB / -4.1162000e-02 -1.0380000e-01 -1.7913000e-02 /
CHEB / -1.6129000e-03 -4.9241000e-02 -2.0058000e-02 /

CH3+nSPC(102)(+m)=C2H5O-3+O(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -29.376765158168332 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1103000e+01 -3.7919000e-04 -2.6400000e-04 /
CHEB / -8.0677000e-02 2.7925000e-04 1.9442000e-04 /
CHEB / 1.7839000e-01 1.5729000e-04 1.0951000e-04 /
CHEB / 6.1360000e-02 -1.0069000e-05 -7.0182000e-06 /
CHEB / -1.3727000e-03 -3.7811000e-05 -2.6328000e-05 /

C2H5O-3+O(+m)=C2H5+O2(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -26.867072671080518 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3488000e+01 -3.9280000e-04 -3.2169000e-04 /
CHEB / -7.1260000e-01 2.4969000e-04 2.1327000e-04 /
CHEB / -1.5083000e-01 2.5674000e-04 2.0672000e-04 /
CHEB / -7.9056000e-02 -4.2323000e-05 -4.2157000e-05 /
CHEB / -4.6028000e-02 -8.4017000e-05 -7.0417000e-05 /

C2H5O-3+O(+m)=C2H4+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C2H5O2) deltaHrxn(T=298K) = -40.3555745979382 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2378000e+01 2.3983000e-03 1.6420000e-03 /
CHEB / 4.1467000e-01 -1.7921000e-03 -1.2303000e-03 /
CHEB / 1.5479000e-01 -1.1218000e-03 -7.5544000e-04 /
CHEB / 3.3601000e-02 7.9585000e-05 4.6799000e-05 /
CHEB / 2.0691000e-03 3.5739000e-04 2.3679000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
```

```
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H7-2            26.01 68.9  16.37 20.25 24.07 27.48 33.07 37.34
      44.11
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C3H7-2+O2(+m)=C3H6+HO2(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -17.378259065589866 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2351000e+01 -6.6552000e-01 -1.7753000e-01 /
CHEB / 3.4807000e-01 8.2364000e-01 1.7173000e-01 /
CHEB / -9.6700000e-02 -5.1798000e-02 6.3394000e-02 /
CHEB / -7.6684000e-02 -1.1780000e-01 -4.4725000e-02 /
CHEB / -9.1991000e-03 -2.0858000e-02 -2.8941000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH2OH             -3.84 58.19 11.45 12.96 14.32 15.46 17.23 18.59
      20.93
!     C3H7O-N2    -13.23      80.42 21.04 25.11 28.98 32.38 37.87 42.05
      48.76
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH3OH             -48.47      57.18 10.59 12.35 14.25 16.01 18.95
      21.25 25.02
!     C3H6O-enol2       -28.93      72.64 21.54 25.01 28.2  31.01 35.6
      39.14 44.92
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
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!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9
!     C3H6O-enol  -34.7 70.85 20.67 24.56 28.02 30.98 35.68 39.25 45.02
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

C3H7O-N2+O2(+m)=C3H6O-enol2+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -13.308921314831693 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1529000e+01 -8.4191000e-01 -1.4304000e-01 /
CHEB / 8.7967000e-01 9.8548000e-01 9.9596000e-02 /
CHEB / -1.0125000e-01 8.7331000e-03 9.7281000e-02 /
CHEB / -9.2293000e-02 -1.4194000e-01 -2.3064000e-02 /
CHEB / -1.7170000e-02 -4.7331000e-02 -3.9362000e-02 /

C3H7O-N2+O2(+m)=C3H6O-enol+HO2(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (test1)  deltaHrxn(T=298K) = -19.078187210445712 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1098000e+01 -9.5705000e-01 -1.5442000e-01 /
CHEB / 7.0329000e-01 1.1184000e+00 1.0463000e-01 /
CHEB / -1.6432000e-01 1.4083000e-02 1.0973000e-01 /
CHEB / -1.1414000e-01 -1.6075000e-01 -2.4733000e-02 /
CHEB / -2.0309000e-02 -5.8786000e-02 -4.5243000e-02 /

C3H6O-enol2+HO2(+m)=C3H6O-enol+HO2(+m)    1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (test1)   deltaHrxn(T=298K) = -5.769265895614023
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.2740000e+00 -1.1979000e+00 -6.4193000e-02 /
CHEB / 4.4068000e+00 1.2581000e+00 -2.8197000e-02 /
CHEB / -2.6752000e-02 2.1069000e-01 1.2109000e-01 /
CHEB / -9.6537000e-02 -1.9385000e-01 2.5674000e-02 /
CHEB / 7.9915000e-03 -1.2972000e-01 -4.3013000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CCCC(OO)OH  -59.56      100.66      33.8  40.53 46.75 51.68 59.24
      65.55 73.72 null
!     CcCC(OOH)OH -49.31      105.57      34.31 40.6  46.81 51.87 59.61
      65.88 74.16 null
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H5              29.43 59.12 12.25 14.77 17.18 19.31 22.84 25.61
      30.13
!     C3H7-1            25.21 69.28 17.39 21.53 25.29 28.54 33.78 37.81
      44.29
```

```
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H9O-4           -23.13      86.3  26.57 32.71 38.13 42.67 49.73
      54.99 63.34  !MRH
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     C2H5OH            -56.24      66.77 15.67 19.24 22.57 25.46 30.09
      33.6  39.27
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     HOCHOOH     -25.83      77.47 18.14 20.12 21.93 23.68 26.4  28.62
      29.35 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H8O-enol        -42.24      81.3  24.52 30.69 35.99 40.36 47.01
      51.87 59.46 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     C4H9O-4+O2=CCCC(OO)OH   3.7700000e+12      0.00000
0.0000000e+00
!     CCCC(OO)OH=CcCC(OOH)OH  3.5760000e+07      1.26000
1.8170000e+04
!     C3H6+HOCHOOH=CcCC(OOH)OH      1.7353374e+11      0.00000
1.0733333e+04
!     CCCC(OO)OH=C4H8O-enol+HO2     6.6000000e+09      1.01000
2.9600000e+04

CcCC(OOH)OH(+m)=CCCC(OO)OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -10.248866762522084
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.7915000e+00 1.0817000e+00 -2.3883000e-01 /
CHEB / -3.9336000e+00 8.2088000e-01 -2.0198000e-02 /
CHEB / -5.4822000e+00 -1.9368000e-01 1.3874000e-02 /
CHEB / -2.2965000e+00 -4.4351000e-01 -8.3901000e-02 /
CHEB / -6.0414000e-01 -2.7676000e-01 -8.0750000e-02 /

C4H9O-4+O2(+m)=CCCC(OO)OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/CsO     O2_birad       deltaHrxn(T=298K) = -
37.10632423842435 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1000000e+00 1.3986000e+00 -2.0993000e-01 /
CHEB / -9.2310000e+00 1.9592000e+00 -2.0042000e-01 /
CHEB / -5.3224000e+00 6.2814000e-01 3.4772000e-02 /
CHEB / -2.5103000e+00 -2.0447000e-01 6.2604000e-02 /
CHEB / -7.5419000e-01 -3.1924000e-01 -8.9859000e-03 /

C4H9O-4+O2(+m)=CcCC(OOH)OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -26.85745747590227
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 9.8118000e+00 8.1595000e-01 -4.2232000e-01 /
CHEB / -5.2333000e+00 2.5844000e+00 3.0219000e-02 /
CHEB / -3.2325000e+00 5.1389000e-01 8.5947000e-02 /
CHEB / -1.9442000e+00 -1.8459000e-01 1.2493000e-02 /
CHEB / -9.1283000e-01 -2.7058000e-01 -1.5010000e-03 /

C3H6+HOCHOOH(+m)=CCCC(OO)OH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -39.965918626736176
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7658000e-01 3.1613000e+00 -1.0130000e+00 /
CHEB / -5.3978000e+00 3.0930000e+00 2.8749000e-01 /
CHEB / -5.5118000e+00 3.2544000e-01 1.8527000e-01 /
CHEB / -2.4444000e+00 -3.8023000e-01 1.4706000e-02 /
CHEB / -6.4669000e-01 -3.6236000e-01 -2.6581000e-02 /

C3H6+HOCHOOH(+m)=CcCC(OOH)OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Cd/H2_Cd/H/Nd     C_rad/H/O2
      deltaHrxn(T=298K) = -29.717051864214092 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.8687000e+00 3.8489000e+00 -8.0880000e-01 /
CHEB / -2.5272000e+00 2.1579000e+00 1.2418000e-01 /
CHEB / -3.2700000e+00 3.0274000e-01 8.0896000e-02 /
CHEB / -1.7557000e+00 -1.3898000e-01 8.6437000e-02 /
CHEB / -7.7458000e-01 -2.4408000e-01 6.1605000e-02 /

C4H9O-4+O2(+m)=C3H6+HOCHOOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = 2.859594388311823
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.5595000e+00 -9.6475000e-01 -3.8088000e-01 /
CHEB / 4.4896000e+00 1.1778000e+00 4.0692000e-01 /
CHEB / -6.0549000e-01 -6.9173000e-02 6.6387000e-02 /
CHEB / -3.9521000e-01 -1.4079000e-01 -7.5181000e-02 /
CHEB / -1.9743000e-01 -4.1814000e-02 -3.8501000e-02 /

C4H8O-enol+HO2(+m)=CCCC(OO)OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -20.38815202979012
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.2063000e+00 1.0420000e+00 -1.2307000e-01 /
CHEB / -3.8010000e+00 1.5416000e+00 -1.3380000e-01 /
CHEB / -4.7317000e+00 5.4825000e-01 8.8350000e-03 /
CHEB / -2.3330000e+00 -1.6366000e-01 4.5010000e-02 /
CHEB / -7.0533000e-01 -2.9365000e-01 -2.6377000e-03 /

C4H8O-enol+HO2(+m)=CcCC(OOH)OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -10.139285267268036
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
```

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CHEB / 2.7299000e+00 3.0190000e-01 -3.0790000e-01 /
CHEB / 4.3971000e-01 2.3369000e+00 3.0151000e-02 /
CHEB / -2.6884000e+00 4.5749000e-01 1.0007000e-01 /
CHEB / -1.7900000e+00 -1.8906000e-01 -2.2664000e-03 /
CHEB / -8.6982000e-01 -2.5926000e-01 -1.5178000e-02 /

C4H9O-4+O2(+m)=C4H8O-enol+HO2(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -16.718172208634233
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.1703000e+01 -1.0270000e+00 -8.7726000e-02 /
CHEB / 7.3859000e-01 1.1079000e+00 2.7689000e-02 /
CHEB / -4.0842000e-02 1.6591000e-01 9.5300000e-02 /
CHEB / -1.4810000e-01 -1.8799000e-01 1.0907000e-02 /
CHEB / -4.2422000e-02 -1.2700000e-01 -4.7276000e-02 /

C3H6+HOCHOOH(+m)=C4H8O-enol+HO2(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (CCCC(OO)OH)   deltaHrxn(T=298K) = -19.577766596946056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9628000e+00 -9.4121000e-01 -3.9300000e-01 /
CHEB / 4.3947000e+00 1.1624000e+00 4.2957000e-01 /
CHEB / -3.5465000e-01 -6.8962000e-02 6.3839000e-02 /
CHEB / -2.9296000e-01 -1.5029000e-01 -8.3251000e-02 /
CHEB / -1.4885000e-01 -5.1966000e-02 -4.5481000e-02 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C4H8-1            1.88  73.18 20.82 26.08 30.86 34.96 41.53 46.49
      54.36
!     C4H9O-3           -18.5 88.73 28.25 33.57 38.32 42.48 49.29 54.55
      63.04  !MRH
!     C4H8-2            -0.84 70.68 21.14 25.96 30.54 34.59 41.2  46.25
      54.24
!Here are the path reactions and their high-P limit kinetics:
!     C4H8-1+C4H9O-3=adduct(1)      2.4800000e+01      2.93000
4.3900000e+04
!     C4H8-2+C4H9O-3=adduct(1)      1.1691492e+02      2.87714
4.8857143e+04

C4H8-2+C4H9O-3(+m)=C4H8-1+C4H9O-3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (adduct)  deltaHrxn(T=298K) = 2.719803185470056
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8157000e+01 -3.8163000e-01 -1.6723000e-01 /
CHEB / 2.2549000e+01 4.8130000e-01 1.9406000e-01 /
CHEB / 1.3470000e+00 -4.5021000e-02 7.9288000e-03 /
CHEB / 2.9545000e-01 -6.5593000e-02 -3.4565000e-02 /
CHEB / 5.6843000e-02 -5.1701000e-03 -1.0164000e-02 /
```

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!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(46)    13.05 89.3  26.98 33.24 38.39 42.37 48.73 53.73 60.56
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH3CH[o]C2H3      12.71 80.32 23.24 29.25 34.38 38.3  44.62 49.1
      55.26 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+C4H7-24=sSPC(46)     3.7700000e+12      0.00000
0.0000000e+00
!     sSPC(46)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04
!     sSPC(46)=HO2+C4H6-13    4.3669559e+09      1.31333
2.9866667e+04
!     CH3CH[o]C2H3+O=sSPC(46) 1.0000000e+13      0.00000
0.0000000e+00

O2+C4H7-24(+m)=C4H6O(717)+OH(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(46))     deltaHrxn(T=298K) = -57.16446243249892
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.5817000e+00 -1.5656000e-02 -1.2626000e-02 /
CHEB / 6.1412000e+00 1.8916000e-02 1.5289000e-02 /
CHEB / 2.1379000e-01 7.3819000e-04 5.0385000e-04 /
CHEB / 9.9143000e-03 -5.3062000e-03 -4.2061000e-03 /
CHEB / -3.3648000e-02 1.6560000e-04 1.4417000e-04 /

CH3CH[o]C2H3+O(+m)=C4H6O(717)+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (sSPC(46))      deltaHrxn(T=298K) = -
94.05056754909889 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
```

```
CHEB / 5    3 /
CHEB / 9.8811000e+00 -1.8747000e-03 -1.3062000e-03 /
CHEB / 1.1029000e+00 1.8294000e-03 1.2747000e-03 /
CHEB / 5.6132000e-01 4.4479000e-04 3.0980000e-04 /
CHEB / 1.1580000e-01 -3.0946000e-04 -2.1576000e-04 /
CHEB / 1.0188000e-02 -1.1645000e-04 -8.1094000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     sSPC(56)    14.62 90.56 26.69 31.95 36.56 40.69 47.29 52.59 60.37
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     C4H7-24           34.78 71.99 19.86 24.81 29.29 33.1  39.1  43.57
      50.6
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     pC3H5             65.51 64.88 15.28 18.48 21.36 23.85 27.84 30.89
      35.74
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6-13           28.95 65.82 18.48 23.96 28.66 32.35 37.56 41.12
      46.59
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     C4H6-12           40.97 69.71 18.95 23.2  27.03 30.32 35.57 39.54
      45.78
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+C4H7-24=sSPC(56)     2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+pC3H5=sSPC(56)      1.4157154e+13      -0.15000
2.9166667e+02
!     sSPC(56)=HO2+C4H6-12    5.8013126e+10      0.62333
3.0055556e+04

HO2+C4H6-13(+m)=sSPC(56)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56))     deltaHrxn(T=298K) = -17.398346582460896
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1284000e+00 2.5482000e+00 -7.1448000e-01 /
CHEB / -9.5430000e-01 2.1481000e+00 5.2545000e-01 /
CHEB / -3.7753000e+00 2.5628000e-01 3.6144000e-01 /
CHEB / -1.9262000e+00 -3.6183000e-01 8.7395000e-02 /
CHEB / -7.3548000e-01 -2.9219000e-01 -5.2523000e-02 /
```

```
nSPC(102)+pC3H5(+m)=HO2+C4H6-13(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (sSPC(56))     deltaHrxn(T=298K) = -84.59114193512227
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2994000e+00 1.4147000e-03 9.9153000e-04 /
CHEB / -2.8241000e-01 -1.0645000e-03 -7.4661000e-04 /
CHEB / -5.0705000e-02 -5.4839000e-04 -3.8498000e-04 /
CHEB / -5.4328000e-02 6.0726000e-05 4.3599000e-05 /
CHEB / -4.3815000e-02 1.2273000e-04 8.6568000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     tSPC(77)    14.04 87.55 29.0  35.14 40.21 44.42 50.74 55.55 62.27
      null
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     iC4H7       35.2  70.24 19.59 24.94 29.51 33.32 39.22 43.62 50.57
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     sC3H5             61.96 65.41 15.14 18.18 21.04 23.56 27.66 30.78
      35.73
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     aC3H4             47.11 59.34 13.97 17.02 19.63 21.79 25.18 27.73
      31.82
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     C4H6O(105)  -2.12 71.03 19.46 26.19 31.81 36.09 42.58 47.31 53.93
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H7OJ(79)  13.7  80.55 23.83 28.87 33.43 37.38 43.75 48.41 55.38
      null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+iC4H7=tSPC(54)       2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+sC3H5=tSPC(54)      1.4157154e+13      -0.15000
2.9166667e+02
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```
!     tSPC(54)=tSPC(77)       1.1250000e+11      0.00000
2.4400000e+04
!     CH2OOH+aC3H4=tSPC(77)   1.9263655e+11      0.04067
9.2900000e+03
!     C4H7OJ(79)+O=tSPC(54)   1.0000000e+13      0.00000
0.0000000e+00

O2+iC4H7(+m)=C4H6O(105)+OH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -29.306965878780556
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.5615000e+01 -3.0891000e-01 5.3010000e-02 /
CHEB / 1.9320000e+01 3.8646000e-01 -8.2150000e-02 /
CHEB / 1.3161000e+00 -3.0965000e-02 2.4777000e-02 /
CHEB / 3.8410000e-01 -4.8229000e-02 1.4570000e-02 /
CHEB / 1.0265000e-01 -1.7345000e-02 -6.0243000e-03 /

nSPC(102)+sC3H5(+m)=C4H6O(105)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (tSPC(54))      deltaHrxn(T=298K) = -
106.4888845355491 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.7891000e+00 -9.9117000e-04 -6.8982000e-04 /
CHEB / 1.1871000e+01 7.2019000e-04 5.0122000e-04 /
CHEB / 9.8335000e-01 3.6695000e-04 2.5538000e-04 /
CHEB / 3.5395000e-01 9.5367000e-06 6.6440000e-06 /
CHEB / 1.0623000e-01 -6.9377000e-05 -4.8276000e-05 /

CH2OOH+aC3H4(+m)=C4H6O(105)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -55.54392132412964
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.2957000e+01 -4.6253000e-01 -1.7037000e-01 /
CHEB / 1.4734000e+01 5.7486000e-01 1.9097000e-01 /
CHEB / 9.2472000e-01 -4.4048000e-02 1.5690000e-02 /
CHEB / 3.0193000e-01 -7.7904000e-02 -3.2350000e-02 /
CHEB / 1.2378000e-01 -8.0684000e-03 -1.3120000e-02 /

O2+iC4H7(+m)=C4H6Oi-13+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -54.52508434966465
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.7768000e+00 -7.3960000e-01 7.7652000e-02 /
CHEB / 5.8107000e+00 8.8520000e-01 -9.8733000e-02 /
CHEB / 3.2074000e-01 -6.9525000e-02 -1.5690000e-02 /
CHEB / 4.8439000e-02 -4.4644000e-02 4.7265000e-02 /
CHEB / 3.3059000e-02 -3.9757000e-02 8.3832000e-03 /

nSPC(102)+sC3H5(+m)=C4H6Oi-13+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (tSPC(54))      deltaHrxn(T=298K) = -
131.70700300643318 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0608000e+01 -3.7295000e-04 -2.5973000e-04 /
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CHEB / 1.2995000e+00 2.5337000e-04 1.7646000e-04 /
CHEB / 3.6488000e-01 1.4696000e-04 1.0235000e-04 /
CHEB / 1.1299000e-01 1.6362000e-05 1.1382000e-05 /
CHEB / 1.9647000e-02 -2.1538000e-05 -1.5009000e-05 /

CH2OOH+aC3H4(+m)=C4H6Oi-13+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -80.76203979501373
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 6.3135000e+00 -5.0718000e-01 -2.0195000e-01 /
CHEB / 3.0026000e+00 5.8829000e-01 2.0867000e-01 /
CHEB / -4.3945000e-02 1.5333000e-02 3.8370000e-02 /
CHEB / -2.9708000e-02 -8.9491000e-02 -2.8822000e-02 /
CHEB / 1.3994000e-02 -2.7895000e-02 -2.3286000e-02 /

tSPC(110)+OH(+m)=tSPC(54)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -20.717514648154296
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.4088000e+01 1.8326000e+00 -3.9741000e-02 /
CHEB / 1.0132000e+01 2.2001000e+00 -3.1303000e-01 /
CHEB / -3.0819000e+00 7.3130000e-01 -5.4781000e-02 /
CHEB / -1.8773000e+00 1.9920000e-01 2.0298000e-01 /
CHEB / -8.1689000e-01 -9.5234000e-02 1.5281000e-01 /

tSPC(110)+OH(+m)=tSPC(77)(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -20.717688480972754
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1715000e+01 1.5649000e+00 -2.5212000e-01 /
CHEB / 9.3039000e+00 2.3072000e+00 -2.1074000e-01 /
CHEB / -3.2640000e+00 9.8663000e-01 9.5435000e-02 /
CHEB / -2.0691000e+00 9.4196000e-02 1.6316000e-01 /
CHEB / -9.4488000e-01 -1.8906000e-01 8.3380000e-02 /

O2+iC4H7(+m)=tSPC(110)+OH(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -1.1204850716839658
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.0277000e+00 -5.5937000e-01 8.0764000e-02 /
CHEB / 1.6188000e+01 6.9493000e-01 -1.1287000e-01 /
CHEB / 7.7976000e-01 -7.6070000e-02 1.1790000e-02 /
CHEB / 2.1486000e-01 -4.4156000e-02 3.1804000e-02 /
CHEB / 7.1870000e-02 -3.3377000e-02 2.4282000e-04 /

nSPC(102)+sC3H5(+m)=tSPC(110)+OH(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (tSPC(54))      deltaHrxn(T=298K) = -
78.3024037284525 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.3818000e+00 -7.1976000e-04 -5.0106000e-04 /
CHEB / 1.0574000e+01 4.9847000e-04 3.4702000e-04 /
CHEB / 5.5838000e-01 2.7715000e-04 1.9294000e-04 /
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CHEB / 1.9732000e-01 2.2078000e-05 1.5359000e-05 /
CHEB / 5.0485000e-02 -4.5191000e-05 -3.1465000e-05 /

CH2OOH+aC3H4(+m)=tSPC(110)+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -27.35744051703305
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.5980000e+00 -4.9833000e-01 -1.8647000e-01 /
CHEB / 1.2779000e+01 5.9318000e-01 1.9901000e-01 /
CHEB / 3.3410000e-01 -9.2337000e-03 2.8271000e-02 /
CHEB / 1.1498000e-01 -8.6330000e-02 -3.0565000e-02 /
CHEB / 6.4916000e-02 -1.8955000e-02 -1.8673000e-02 /

C4H7OJ(79)+O(+m)=C4H6O(105)+OH(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -66.76280864724777
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.8099000e+00 -2.0927000e-02 -1.0261000e-02 /
CHEB / 1.3396000e+01 2.5209000e-02 1.1388000e-02 /
CHEB / 1.4418000e+00 -1.3875000e-03 7.3419000e-04 /
CHEB / 4.4635000e-01 -3.2068000e-03 -1.7233000e-03 /
CHEB / 1.1334000e-01 -2.7482000e-04 -5.1138000e-04 /

C4H7OJ(79)+O(+m)=C4H6Oi-13+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -91.98092711813186
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.0126000e+01 -2.0994000e-02 -1.0308000e-02 /
CHEB / 1.8652000e+00 2.3955000e-02 1.0809000e-02 /
CHEB / 5.5976000e-01 7.9874000e-04 1.5788000e-03 /
CHEB / 1.6892000e-01 -3.6439000e-03 -1.5721000e-03 /
CHEB / 3.7654000e-02 -8.2693000e-04 -8.6092000e-04 /

C4H7OJ(79)+O(+m)=tSPC(110)+OH(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (tSPC(54))     deltaHrxn(T=298K) = -38.576327840151166
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.6225000e+00 -2.1784000e-02 -1.0357000e-02 /
CHEB / 1.1559000e+01 2.5352000e-02 1.1034000e-02 /
CHEB / 8.9130000e-01 -6.7522000e-05 1.3270000e-03 /
CHEB / 2.8311000e-01 -3.5504000e-03 -1.6326000e-03 /
CHEB / 6.8184000e-02 -6.2106000e-04 -7.3826000e-04 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(97)    -58.6 98.35 33.06 40.41 46.39 51.35 59.12 65.16 72.32
      null
!     tSPC(439)   -45.7 101.55      34.34 41.89 48.03 53.04 60.68 66.39
      72.74 null
```

```
!     O2                0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24
      8.58
!     HOC[CH2][CH3]2    -24.74      81.5  29.21 35.23 40.22 44.31 50.69
      55.53 63.46  !MRH
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     nSPC(102)   51.11 64.1  13.19 14.68 15.86 17.01 18.79 20.57 23.05
      null
!     CH3C[OH]CH3 -22.33      74.56 21.77 26.05 29.95 33.3  38.64 42.68
      49.13
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     tSPC(54)    14.04 89.53 27.57 32.86 37.44 41.45 47.86 53.04 60.68
      null
!     H2O               -58.46      45.02 7.99  8.15  8.37  8.63  9.17
      9.73  11.01
!     CH2OOH      15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54 28.13
      null
!     H2CCCH3[OH] -39.44      69.6  20.59 25.3  29.06 32.04 36.55 39.89
      45.32
!     C4H8O2(62)  -22.06      89.31 29.62 35.7  40.99 45.54 52.58 58.01
      65.76 null
!     HO2               3.07  54.61 8.28  8.82  9.38  9.88  10.66 11.26
      12.25
!     sSPC(1474)  -67.94      85.82 28.37 33.77 38.22 41.77 46.97 50.61
      56.09
!     acetone     -51.21      70.9  17.53 21.65 25.52 28.9  34.34 38.41
      44.77
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     O2+HOC[CH2][CH3]2=tSPC(97)    2.2600000e+12      0.00000
0.0000000e+00
!     nSPC(102)+CH3C[OH]CH3=tSPC(97)      3.5900000e+14      -0.75000
0.0000000e+00
!     tSPC(54)+H2O=tSPC(97)   1.2500000e+03      2.76000
4.8500000e+04
!     tSPC(97)=tSPC(439)      5.0760000e+08      1.32000
2.1500000e+04
!     CH2OOH+H2CCCH3[OH]=tSPC(439)  2.4827386e+10      0.24400
1.0487500e+04
!     C4H8O2(62)+OH=tSPC(439) 2.7100000e+12      0.00000
0.0000000e+00

sSPC(1474)+CH3(+m)=tSPC(97)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -25.906753483188908
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -8.6645000e+00 2.5902000e+00 -4.3612000e-01 /
CHEB / 4.0913000e+00 2.3474000e+00 6.8205000e-02 /
CHEB / -3.8299000e+00 4.2502000e-01 1.5135000e-01 /
CHEB / -2.3140000e+00 -2.9434000e-01 6.8232000e-02 /
CHEB / -9.8283000e-01 -2.7098000e-01 -4.4833000e-03 /
```

```
sSPC(1474)+CH3(+m)=tSPC(439)(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -13.008239732306244
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -9.7917000e+00 2.8023000e+00 -3.1995000e-01 /
CHEB / 6.2240000e+00 2.0714000e+00 -7.2646000e-02 /
CHEB / -2.7350000e+00 3.9439000e-01 1.1614000e-01 /
CHEB / -1.9266000e+00 -1.9357000e-01 1.2735000e-01 /
CHEB / -1.0609000e+00 -2.3912000e-01 1.9011000e-02 /

O2+HOC[CH2][CH3]2(+m)=sSPC(1474)+CH3(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
8.62935701826077 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 3.0910000e-01 -6.1700000e-01 -1.9189000e-01 /
CHEB / 9.1606000e+00 7.6083000e-01 1.8583000e-01 /
CHEB / 6.4592000e-01 -4.9466000e-02 6.5795000e-02 /
CHEB / -4.9893000e-02 -1.0100000e-01 -4.5530000e-02 /
CHEB / -6.0329000e-02 -1.7426000e-02 -2.9179000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=sSPC(1474)+CH3(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -61.464187836958665 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.3871000e+00 -7.1434000e-02 -4.9895000e-02 /
CHEB / 1.4134000e+00 8.8752000e-02 6.1796000e-02 /
CHEB / 6.1179000e-01 -7.2636000e-03 -4.6909000e-03 /
CHEB / 1.3674000e-01 -1.1603000e-02 -8.2950000e-03 /
CHEB / -3.4561000e-02 -9.7596000e-04 -7.2784000e-04 /

sSPC(1474)+CH3(+m)=tSPC(54)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -11.728549837843403
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.1349000e+01 -3.6384000e-01 -1.8451000e-01 /
CHEB / 1.7399000e+01 4.5086000e-01 2.1739000e-01 /
CHEB / 1.0366000e+00 -3.2824000e-02 1.0626000e-03 /
CHEB / 2.2809000e-01 -6.2752000e-02 -3.4867000e-02 /
CHEB / 1.9106000e-02 -4.9308000e-03 -7.2446000e-03 /

CH2OOH+H2CCCH3[OH](+m)=sSPC(1474)+CH3(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
8.259481691212784 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -3.0928000e+00 -4.1299000e-01 -1.0880000e-01 /
CHEB / 1.0661000e+01 5.3498000e-01 1.0961000e-01 /
CHEB / 6.8543000e-01 -9.4300000e-02 2.4714000e-02 /
CHEB / 2.8956000e-02 -2.1227000e-02 -1.4724000e-02 /
CHEB / -4.2268000e-02 -1.6594000e-02 -1.6891000e-02 /
```

```
C4H8O2(62)+OH(+m)=sSPC(1474)+CH3(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
19.31818680818852 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.8835000e+00 -4.1299000e-01 -1.0880000e-01 /
CHEB / 6.7294000e+00 5.3498000e-01 1.0961000e-01 /
CHEB / 6.5074000e-01 -9.4300000e-02 2.4714000e-02 /
CHEB / 1.4319000e-02 -2.1227000e-02 -1.4724000e-02 /
CHEB / -5.1740000e-02 -1.6594000e-02 -1.6891000e-02 /

CH2OOH+acetone(+m)=tSPC(97)(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -22.39781690489015
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -7.4000000e+00 2.3277000e+00 -4.1382000e-01 /
CHEB / 4.6612000e+00 2.1601000e+00 5.1897000e-02 /
CHEB / -3.8956000e+00 4.6774000e-01 1.2335000e-01 /
CHEB / -2.3503000e+00 -2.6963000e-01 6.3020000e-02 /
CHEB / -1.0201000e+00 -2.7652000e-01 -2.6076000e-03 /

tSPC(439)(+m)=CH2OOH+acetone(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = 9.499303154007485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0132000e+01 2.5276000e+00 -3.0790000e-01 /
CHEB / 9.2991000e+00 1.9011000e+00 -7.4775000e-02 /
CHEB / -3.0341000e+00 4.3515000e-01 8.6561000e-02 /
CHEB / -2.0209000e+00 -1.7570000e-01 1.1637000e-01 /
CHEB / -1.0985000e+00 -2.3979000e-01 2.4961000e-02 /

O2+HOC[CH2][CH3]2(+m)=CH2OOH+acetone(+m)  1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
12.138293596559521 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.9064000e+00 -6.7448000e-01 -1.8977000e-01 /
CHEB / 7.8038000e+00 8.0790000e-01 1.7086000e-01 /
CHEB / 3.4651000e-01 -1.9922000e-02 7.8067000e-02 /
CHEB / -1.5351000e-01 -1.1384000e-01 -3.6527000e-02 /
CHEB / -1.1042000e-01 -2.5308000e-02 -3.5204000e-02 /

nSPC(102)+CH3C[OH]CH3(+m)=CH2OOH+acetone(+m)    1.0E0 0.0 0.0
      !NetReaction from PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K)
= -64.97312441525742 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3678000e+00 -6.3472000e-02 -4.5491000e-02 /
CHEB / 5.2768000e-01 7.9252000e-02 5.6688000e-02 /
CHEB / 3.2270000e-01 -6.9176000e-03 -4.6893000e-03 /
CHEB / 3.8951000e-02 -1.0308000e-02 -7.5767000e-03 /
CHEB / -6.4843000e-02 -8.4602000e-04 -6.2068000e-04 /
```

```
CH2OOH+acetone(+m)=tSPC(54)+H2O(+m) 1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (tSPC(97))     deltaHrxn(T=298K) = -8.219613259544644
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.0833000e+01 -3.7452000e-01 -1.8882000e-01 /
CHEB / 1.7880000e+01 4.5680000e-01 2.1855000e-01 /
CHEB / 8.2853000e-01 -2.3226000e-02 6.2347000e-03 /
CHEB / 1.2011000e-01 -6.4916000e-02 -3.5062000e-02 /
CHEB / -2.9425000e-02 -8.4522000e-03 -9.2047000e-03 /

CH2OOH+H2CCCH3[OH](+m)=CH2OOH+acetone(+m) 1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
11.768418269511542 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -6.2287000e-01 -4.8268000e-01 -1.1710000e-01 /
CHEB / 9.3647000e+00 6.1997000e-01 1.1533000e-01 /
CHEB / 3.8096000e-01 -1.0416000e-01 2.6422000e-02 /
CHEB / -7.9137000e-02 -2.5659000e-02 -9.7052000e-03 /
CHEB / -7.9080000e-02 -1.5192000e-02 -1.9583000e-02 /

C4H8O2(62)+OH(+m)=CH2OOH+acetone(+m)      1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
22.827123386487276 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.3534000e+00 -4.8268000e-01 -1.1710000e-01 /
CHEB / 5.4335000e+00 6.1997000e-01 1.1533000e-01 /
CHEB / 3.4628000e-01 -1.0416000e-01 2.6422000e-02 /
CHEB / -9.3774000e-02 -2.5659000e-02 -9.7052000e-03 /
CHEB / -8.8553000e-02 -1.5192000e-02 -1.9583000e-02 /

sSPC(1474)+CH3(+m)=CH2OOH+acetone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (tSPC(97))      deltaHrxn(T=298K) = -
3.5089365782987585 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 5.8232000e+00 -5.5171000e-04 -4.4838000e-04 /
CHEB / 3.7551000e+00 7.5048000e-04 6.1001000e-04 /
CHEB / -8.2179000e-02 -1.1658000e-04 -9.5036000e-05 /
CHEB / -3.9731000e-02 -1.6857000e-04 -1.3679000e-04 /
CHEB / -4.6552000e-02 8.5859000e-05 6.9933000e-05 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     C6H10       20.18 89.38 28.76 36.5  43.28 48.98 57.88 64.4  74.34
      null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C2H3             72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
```

```
!     C4H7-14           48.89 77.02 19.8  24.73 29.13 32.88 38.8  43.23
      50.09 null
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6
!     C6H9_1_2_5  53.64 88.19 27.85 35.53 41.96 47.27 55.5  61.53 70.54
      null
!Here are the path reactions and their high-P limit kinetics:
!     C2H3+C4H7-14=C6H10      1.4157154e+13      -0.15000
2.9166667e+02
!     aC3H5+aC3H5=C6H10       1.1500000e+13      0.00000
0.0000000e+00
!     C6H9_1_2_5+H=C6H10      5.0000000e+13      0.00000
0.0000000e+00

C2H3+C4H7-14(+m)=C6H10(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10) High-P Limit: R_Recombination estimate:
(Average:) Cd_pri_rad     C_rad/H2/Cs           deltaHrxn(T=298K) = -
100.89962492111346 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2026000e+01 1.1165000e+00 -2.2195000e-01 /
CHEB / -1.8445000e+00 7.4913000e-01 1.2315000e-01 /
CHEB / -7.5417000e-01 2.3313000e-01 9.3746000e-02 /
CHEB / -2.6118000e-01 -2.3826000e-02 3.0322000e-02 /
CHEB / -4.1326000e-02 -6.6301000e-02 -1.1652000e-02 /

aC3H5+aC3H5(+m)=C6H10(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H2/Cd     C_rad/H2/Cd          deltaHrxn(T=298K) = -
63.89347015185981 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3557000e+01 3.9795000e-01 -3.9345000e-02 /
CHEB / -1.6986000e+00 7.1278000e-01 -6.1093000e-02 /
CHEB / -6.9512000e-01 5.0472000e-01 -2.1111000e-02 /
CHEB / -4.3023000e-01 2.6562000e-01 1.4662000e-02 /
CHEB / -2.1862000e-01 8.0240000e-02 2.8275000e-02 /

C2H3+C4H7-14(+m)=aC3H5+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10)  deltaHrxn(T=298K) = -37.006154769253634 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2641000e+01 -8.0607000e-01 -2.1059000e-01 /
CHEB / 1.3196000e-01 7.7482000e-01 1.4686000e-01 /
CHEB / 7.7778000e-02 1.7035000e-01 9.1374000e-02 /
CHEB / -5.4054000e-02 -7.0999000e-02 9.7293000e-03 /
CHEB / -4.4033000e-02 -7.3710000e-02 -2.6200000e-02 /

C6H9_1_2_5+H(+m)=C6H10(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10) High-P Limit: R_Recombination estimate:
(Average:) C_rad/H/OneDeC     H_rad       deltaHrxn(T=298K) = -
85.55079330439278 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2909000e+01 6.8557000e-01 -1.0636000e-01 /
CHEB / -1.2893000e+00 9.4293000e-01 -4.0513000e-02 /
CHEB / -7.8234000e-01 4.1481000e-01 6.2147000e-02 /
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CHEB / -3.3368000e-01 6.1296000e-02 6.8459000e-02 /
CHEB / -8.7478000e-02 -6.4599000e-02 2.5822000e-02 /

C6H9_1_2_5+H(+m)=C2H3+C4H7-14(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10)  deltaHrxn(T=298K) = 15.348831616720659 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.8196000e+00 -7.3216000e-01 -2.0550000e-01 /
CHEB / 7.2224000e+00 7.6098000e-01 1.6327000e-01 /
CHEB / 5.3557000e-01 1.0467000e-01 8.2511000e-02 /
CHEB / 5.5658000e-02 -9.0066000e-02 -7.5953000e-03 /
CHEB / -7.7545000e-03 -6.1187000e-02 -3.0810000e-02 /

C6H9_1_2_5+H(+m)=aC3H5+aC3H5(+m)    1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C6H10)  deltaHrxn(T=298K) = -21.65732315253298 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2493000e+01 -1.1771000e+00 -1.1160000e-01 /
CHEB / 1.2584000e+00 1.0359000e+00 -4.5076000e-03 /
CHEB / 1.8441000e-01 3.2103000e-01 9.6460000e-02 /
CHEB / -9.8151000e-02 -5.0961000e-02 5.7880000e-02 /
CHEB / -6.9822000e-02 -1.0933000e-01 -5.8716000e-03 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     C2H3              72.2  55.78 10.41 12.28 13.89 15.23 17.38 19.05
      21.77
!     C4H6O(717)  -30.4 76.82 21.21 26.31 30.83 34.59 40.44 44.92 50.63
      null
!     OH                8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     CH3C[OH]CHcH2     -10.58      79.45 23.81 29.21 33.69 37.49 43.71
      48.21 54.89 null
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:

CH3C[OH]CHcH2+O(+m)=C4H6O(717)+OH(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #3 (C4H7O2J(343))  deltaHrxn(T=298K) = -
70.76279402833872 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.2248000e+01 -5.1029000e-06 -3.5520000e-06 /
CHEB / -1.7868000e-01 -5.3936000e-06 -3.7543000e-06 /
CHEB / -2.4144000e-01 -1.1709000e-06 -8.1500000e-07 /
CHEB / -5.8065000e-03 -5.1798000e-07 -3.6055000e-07 /
CHEB / 1.9594000e-02 -1.4952000e-07 -1.0408000e-07 /

!PDepNetwork
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!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     tSPC(110)   26.07 76.19 23.57 28.7  32.99 36.51 41.99 46.0  52.14
      null
!     C4H6O(105)  -2.12 71.03 19.46 26.19 31.81 36.09 42.58 47.31 53.93
      null
!     C4H6Oi-13   -27.34      74.64 23.14 28.34 32.66 36.17 41.73 45.56
      50.39 null
!     C3H6              6.24  63.59 15.33 19.03 22.5  25.54 30.44 34.19
      40.14
!     CO                -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     CH2               93.85 46.59 8.3   8.66  8.98  9.28  9.87  10.47
      11.69
!     C3H4O-enone       -13.82      68.58 16.45 19.54 22.36 24.81 28.75
      31.71 36.31
!     C3H3O-enone 24.52 67.91 15.61 18.59 21.17 23.32 26.65 29.05 32.71
!     CH3               35.25 46.44 9.36  10.11 10.85 11.55 12.86 14.03
      16.21
!     iC4H5OJ(14) 14.08 76.7  22.34 26.71 30.14 32.93 37.32 40.67 46.0
!MRH CBS-QB3 w/1DHR corrections
!     H                 52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     tSPC(346)   46.45 70.26 16.31 19.12 21.61 23.72 27.02 29.41 32.99
!     iC4H5OJ(15) 12.77 74.84 22.08 26.8  30.77 34.04 39.05 42.66 48.02
!MRH CBS-QB3 w/1DHR corrections
!     O                 59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     tSPC(346)+CH3=tSPC(110) 1.5800000e+11      0.00000
4.9700000e+03
!     iC4H5OJ(14)+H=tSPC(110) 5.2263889e+12      0.04600
5.0666667e+03
!     iC4H5OJ(15)+H=tSPC(110) 1.0000000e+13      0.00000
1.2000000e+03
!     tSPC(110)=C4H6O(105)    5.8853831e+11      0.02483
1.8800000e+03
!     tSPC(110)=C4H6Oi-13     1.2640000e+08      0.00000
0.0000000e+00

CH2+C3H4O-enone(+m)=tSPC(346)+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6OJJ(395))  deltaHrxn(T=298K) =
1.6696942327397295 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.0740000e+01 -3.2394000e-03 -2.2489000e-03 /
CHEB / 2.3873000e+01 4.0309000e-03 2.7970000e-03 /
CHEB / 1.2425000e+00 -4.9932000e-04 -3.4442000e-04 /
CHEB / 2.9886000e-01 -3.0384000e-04 -2.1154000e-04 /
CHEB / 7.2965000e-02 -3.2974000e-05 -2.3194000e-05 /

tSPC(346)+CH3(+m)=C3H3O-enone+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6OJJ(395))  deltaHrxn(T=298K) = -
21.927675029862264 kcal/mol
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```
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8053000e+01 -3.0156000e-03 -2.0943000e-03 /
CHEB / 2.1653000e+01 3.6286000e-03 2.5189000e-03 /
CHEB / 9.8651000e-01 -2.9271000e-04 -2.0159000e-04 /
CHEB / 2.3625000e-01 -3.0663000e-04 -2.1324000e-04 /
CHEB / 4.2512000e-02 -5.0056000e-05 -3.5058000e-05 /

iC4H5OJ(15)+H(+m)=CH2+C3H4O-enone(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6OJJ(395))  deltaHrxn(T=298K) =
15.15878872591098 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.2019000e+01 -2.1804000e-03 -1.5156000e-03 /
CHEB / 2.6807000e+01 2.6169000e-03 1.8185000e-03 /
CHEB / 9.1765000e-01 -2.0933000e-04 -1.4468000e-04 /
CHEB / 2.0936000e-01 -2.0166000e-04 -1.4034000e-04 /
CHEB / 4.2710000e-02 -4.9468000e-05 -3.4516000e-05 /

iC4H5OJ(15)+H(+m)=C3H3O-enone+CH3(+m)     1.0E0 0.0 0.0     !NetReaction
from PDepNetwork #1 (C4H6OJJ(395))  deltaHrxn(T=298K) = -
5.099192071211554 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.8267000e+01 -2.9877000e-03 -2.0750000e-03 /
CHEB / 2.3750000e+01 3.6299000e-03 2.5198000e-03 /
CHEB / 1.0352000e+00 -3.6891000e-04 -2.5439000e-04 /
CHEB / 1.9061000e-01 -2.5363000e-04 -1.7656000e-04 /
CHEB / 1.4979000e-02 -4.4339000e-05 -3.1031000e-05 /

CH2+C3H4O-enone(+m)=C4H6O(105)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6OJJ(395)) deltaHrxn(T=298K) = -82.1408332374233
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.6041000e+01 6.5633000e-05 4.5603000e-05 /
CHEB / 2.0655000e+01 -7.6137000e-06 -5.2107000e-06 /
CHEB / 6.9880000e-01 -3.0182000e-05 -2.1003000e-05 /
CHEB / 1.7388000e-01 -2.3940000e-05 -1.6670000e-05 /
CHEB / 3.1636000e-02 -7.3756000e-06 -5.1415000e-06 /

C3H3O-enone+CH3(+m)=C4H6O(105)(+m)  1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6OJJ(395)) deltaHrxn(T=298K) = -61.88285244030075
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9670000e+01 1.9319000e-05 1.3434000e-05 /
CHEB / 2.3669000e+01 1.8504000e-05 1.2884000e-05 /
CHEB / 7.5703000e-01 -6.1713000e-06 -4.2854000e-06 /
CHEB / 1.4841000e-01 -1.4978000e-05 -1.0422000e-05 /
CHEB / 1.6373000e-02 -1.1320000e-05 -7.8811000e-06 /

CH2+C3H4O-enone(+m)=C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6OJJ(395)) deltaHrxn(T=298K) = -107.35895170830739
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
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CHEB / -1.9779000e+01 6.5633000e-05 4.5603000e-05 /
CHEB / 2.0643000e+01 -7.6137000e-06 -5.2107000e-06 /
CHEB / 6.9582000e-01 -3.0182000e-05 -2.1003000e-05 /
CHEB / 1.7284000e-01 -2.3940000e-05 -1.6670000e-05 /
CHEB / 3.1225000e-02 -7.3756000e-06 -5.1415000e-06 /

C3H3O-enone+CH3(+m)=C4H6Oi-13(+m)   1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #1 (C4H6OJJ(395)) deltaHrxn(T=298K) = -87.10097091118485
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.3408000e+01 1.9319000e-05 1.3434000e-05 /
CHEB / 2.3658000e+01 1.8504000e-05 1.2884000e-05 /
CHEB / 7.5405000e-01 -6.1713000e-06 -4.2854000e-06 /
CHEB / 1.4736000e-01 -1.4978000e-05 -1.0422000e-05 /
CHEB / 1.5962000e-02 -1.1320000e-05 -7.8811000e-06 /

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CHCCCHOH    75.69 76.2  21.5  25.07 27.73 29.93 32.81 34.84 38.89
      null
!     H                52.1  27.36 4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!     C3H2             120.52      62.42 13.2  15.02 16.44 17.7  19.48
      20.84 24.88 null
!     HCO              10.08 53.51 8.25  8.68  9.18  9.68  10.6  11.34
      12.47
!     C2H              137.14      51.64 10.34 10.64 10.89 11.15 11.7
      12.22 13.21
!     pC3H3            86.21 60.63 14.9  17.21 19.0  20.43 22.68 24.42
      27.32
!     CO               -26.44      47.14 6.95  6.99  7.09  7.24  7.57
      7.87  8.34
!     C4H2             113.13      59.15 17.18 19.78 21.53 22.84 24.83
      26.35 28.87
!     OH               8.69  42.53 6.95  6.95  6.95  6.97  7.07  7.23
      7.72
!     nC4H3            132.99      67.35 17.24 20.41 22.8  24.66 27.47
      29.56 32.87
!     O                59.64 36.4  4.96  4.96  4.96  4.96  4.96  4.96
      4.96
!Here are the path reactions and their high-P limit kinetics:
!     C4H2+OH=CHCCCHOH        7.6000000e+07      1.70000
1.0000000e+03

C3H2+HCO(+m)=CHCCCHOH(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -54.904464879833014
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 2.7338000e+00 8.3139000e+00 -1.3968000e+00 /
CHEB / -5.2360000e+00 1.5295000e+00 1.3031000e+00 /
CHEB / -2.2670000e+00 -4.2005000e-01 6.4526000e-01 /
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CHEB / -9.9612000e-01 -4.2869000e-01 1.8479000e-01 /
CHEB / -4.9565000e-01 -1.6365000e-01 3.6590000e-03 /

CHCCCHOH(+m)=pC3H3+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -15.918519849764618
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -2.1247000e+01 8.8714000e+00 -1.4059000e+00 /
CHEB / 1.4541000e+01 1.3636000e+00 1.4005000e+00 /
CHEB / -2.2359000e+00 -5.2343000e-01 6.6805000e-01 /
CHEB / -9.8032000e-01 -4.6251000e-01 1.8289000e-01 /
CHEB / -4.8683000e-01 -1.6277000e-01 -4.6353000e-03 /

C3H2+HCO(+m)=pC3H3+CO(+m)     1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -70.82298472959764
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 7.8349000e+00 -3.2774000e-01 -1.5532000e-01 /
CHEB / 2.6780000e+00 4.0337000e-01 1.7745000e-01 /
CHEB / 3.6201000e-01 -3.6921000e-02 3.4054000e-03 /
CHEB / 5.7645000e-02 -4.0479000e-02 -2.3050000e-02 /
CHEB / 7.8384000e-03 -5.5562000e-03 -6.7457000e-03 /

C4H2+OH(+m)=CHCCCHOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1) High-P Limit: R_Addition_MultipleBond
estimate: (Average:) Ct/H_Ct/De     O_pri_rad         deltaHrxn(T=298K)
= -46.1249189591951 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.2650000e+00 6.8356000e+00 -9.1622000e-01 /
CHEB / -3.9937000e+00 1.2864000e+00 5.7576000e-01 /
CHEB / -1.9001000e+00 -7.4989000e-02 4.9601000e-01 /
CHEB / -8.1120000e-01 -2.3094000e-01 2.4101000e-01 /
CHEB / -3.9063000e-01 -1.3421000e-01 7.7217000e-02 /

C4H2+OH(+m)=C3H2+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = 8.779545920637924
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.2628000e+00 -5.3040000e-01 -2.6561000e-01 /
CHEB / 4.1146000e+00 6.3196000e-01 2.9633000e-01 /
CHEB / 6.2601000e-02 -3.4103000e-02 1.1240000e-02 /
CHEB / -4.7044000e-02 -6.4279000e-02 -3.4564000e-02 /
CHEB / -2.8275000e-02 -1.3788000e-02 -1.2961000e-02 /

C4H2+OH(+m)=pC3H3+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -62.04343880895972
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 4.9362000e+00 -4.7432000e-01 -2.4898000e-01 /
CHEB / 5.8156000e+00 5.6827000e-01 2.8223000e-01 /
CHEB / 3.2548000e-01 -3.4487000e-02 4.7086000e-03 /
CHEB / 6.1689000e-02 -5.7755000e-02 -3.2453000e-02 /
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CHEB / 1.5977000e-02 -1.1296000e-02 -1.0869000e-02 /

nC4H3+O(+m)=CHCCCHOH(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -116.92808721318197
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / -1.9632000e+01 1.7228000e+01 3.0795000e+00 /
CHEB / -4.8182000e+00 -3.5191000e+00 1.0328000e-01 /
CHEB / -1.8002000e+00 -1.0629000e+00 -4.5568000e-01 /
CHEB / -7.5119000e-01 -3.8105000e-01 -1.6251000e-01 /
CHEB / -4.3521000e-01 -1.9591000e-01 8.4688000e-02 /

nC4H3+O(+m)=C3H2+HCO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -62.023622333348946
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 1.3072000e+01 -1.1493000e-07 -7.8472000e-08 /
CHEB / -6.2942000e-02 -5.3738000e-08 -3.9002000e-08 /
CHEB / -7.0550000e-03 4.8698000e-08 3.3652000e-08 /
CHEB / 8.0755000e-03 4.3184000e-08 3.0302000e-08 /
CHEB / 1.2568000e-03 1.0784000e-08 7.6029000e-09 /

nC4H3+O(+m)=pC3H3+CO(+m)      1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #19 (adduct1)     deltaHrxn(T=298K) = -132.8466070629466
kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.3824000e+00 -3.1543000e-06 -2.1948000e-06 /
CHEB / 1.0572000e+00 1.5021000e-06 1.0447000e-06 /
CHEB / 2.9592000e-01 1.4233000e-06 9.9067000e-07 /
CHEB / 1.1578000e-01 3.2859000e-07 2.2891000e-07 /
CHEB / 4.3766000e-02 -9.9388000e-08 -6.9135000e-08 /

nC4H3+O(+m)=C4H2+OH(+m) 1.0E0 0.0 0.0     !NetReaction from PDepNetwork
#19 (adduct1)     deltaHrxn(T=298K) = -70.80316825398687 kcal/mol
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB / 9.1630000e+00 -1.4115000e-03 -1.0223000e-03 /
CHEB / 1.0460000e+00 1.7313000e-03 1.2652000e-03 /
CHEB / 1.5972000e-01 -2.0200000e-04 -1.6466000e-04 /
CHEB / 3.8908000e-02 -1.0609000e-04 -7.0589000e-05 /
CHEB / 7.7147000e-03 -1.8677000e-05 -1.2425000e-05 /

!The following vinoxy + O2 pressure-dependent kinetics are from:
!     J. Lee and J.W. Bozzelli, J. Phys. Chem. A 107 (2003) 3778-3791
CH2CHO+O2=nSPC(543) 1.0 0.0   0.0
PLOG / 0.01 1.58E+77 -21.90 19.35e+03 /
PLOG / 0.1 3.88E+69 -18.84 19.24e+03 /
PLOG / 1 7.80E+59 -15.40 17.65e+03 /
PLOG / 10 3.05E+50 -12.20 15.63e+03 /

CH2CHO+O2=CH2CO+HO2     1.0   0.0   0.0
PLOG / 0.01 1.88E+05 2.37 23.73e+03 /
PLOG / 0.1 1.88E+05 2.37 23.73e+03 /
PLOG / 1 2.51E+05 2.33 23.80e+03 /
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PLOG / 10 7.05E+07 1.63 25.29e+03 /

CH2CHO+O2=CO+CH2O+OH    1.0   0.0   0.0
PLOG / 0.01 2.68E+17 -1.84 6.53e+03 /
PLOG / 0.1 1.52E+20 -2.58 8.98e+03 /
PLOG / 1 1.65E+19 -2.22 10.34e+03 /
PLOG / 10 8.95E+13 -0.60 10.12e+03 /

CH2CHO+O2=HOOCH2CO      1.0   0.0   0.0
PLOG / 0.01 3.64E+65 -21.87 19.02e+03 /
PLOG / 0.1 3.64E+58 -19.00 19.09e+03 /
PLOG / 1 6.65E+48 -15.55 17.46e+03 /
PLOG / 10 4.80E+38 -12.14 14.96e+03 /

nSPC(543)=HOOCH2CO      1.0   0.0   0.0
PLOG / 0.01 8.27E+30 -6.65 24.50e+03 /
PLOG / 0.1 1.73E+26 -4.99 23.76e+03 /
PLOG / 1 9.03E+19 -2.92 22.17e+03 /
PLOG / 10 1.43E+16 -1.67 21.21e+03 /

nSPC(543)=CH2CO+HO2     1.0   0.0   0.0
PLOG / 0.01 2.05E+40 -13.31 52.15e+03 /
PLOG / 0.1 5.72E+45 -14.00 52.20e+03 /
PLOG / 1 4.16E+55 -15.76 55.08e+03 /
PLOG / 10 1.12E+61 -16.04 60.01e+03 /

HOOCH2CO=CO+CH2O+OH     1.0   0.0   0.0
PLOG / 0.01 2.36E+17 -2.95 8.10e+03 /
PLOG / 0.1 2.38E+18 -2.95 8.10e+03 /
PLOG / 1 2.51E+19 -2.95 8.11e+03 /
PLOG / 10 4.16E+20 -3.02 8.24e+03 /

HOOCH2CO=CH2CO+HO2      1.0   0.0   0.0
PLOG / 0.01 1.12E+07 -3.76 21.68e+03 /
PLOG / 0.1 1.10E+08 -3.76 21.68e+03 /
PLOG / 1 9.20E+08 -3.73 21.63e+03 /
PLOG / 10 2.09E+09 -3.55 21.22e+03 /

!MRH 17-May-2011
!Replacing 1993 Bozzelli aC3H5+O2 => CH2O+CH2CHO / C2H2+CH2O+OH
!Note: This assumes CH2OOH does not immediately fall apart to CH2O+OH.
!     That reaction's k(T,P) kinetics is accounted for in the mechanism

!PDepNetwork
!     deltaEdown = 5.514552177052681 kJ/mol
!     bathgas MW = 28.01 amu
!     bathgas LJ sigma = 3.681E-10 meters
!     bathgas LJ epsilon = 1.263615E-21 Joules
!Here are the species and their thermochemistry:
!     CH2CHCH2OO(1)     24.09 80.56 21.15 25.43 29.2  32.34 37.16 40.67
      46.07 Primary Thermo Library: CFG (Species ID: allylperoxy)
!     CHCHCH2OOH(2)     46.9  84.3  23.6  27.44 30.82 33.62 37.87 40.95
      45.74 Primary Thermo Library: MRH (Species ID: CHCHCH2OOH)
!     CH2cyCHCH2OO(3)   39.69 73.94 20.78 25.83 30.04 33.42 38.44 41.99
      47.34 Primary Thermo Library: MRH (Species ID: CH2cyCHCH2OO)
!     aC3H5             42.04 61.54 14.89 18.72 21.97 24.63 28.72 31.76
      36.6  Primary Thermo Library: CFG (Species ID: allyl)
```

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!     O2          0.68  46.74 7.0   7.15  7.37  7.59  7.97  8.24  8.58
      Primary Thermo Library: CFG (Species ID: O2)
!     C2H2              56.1  47.73 10.27 11.79 12.85 13.67 14.94 15.97
      17.79 Primary Thermo Library: CFG (Species ID: C2H2)
!     CH2OOH            15.01 63.88 15.24 17.52 19.41 21.1  23.51 25.54
      28.13 Estimated by Group Additivity
!     CH2CHO            4.75  61.85 12.72 15.28 17.49 19.32 22.13 24.19
      27.35 Primary Thermo Library: CFG (Species ID: vinoxy)
!     CH2O              -26.22      52.16 8.44  9.33  10.38 11.42 13.25
      14.69 16.9  Primary Thermo Library: CFG (Species ID: CH2O)
!Here are the path reactions and their high-P limit kinetics:
!     aC3H5+O2=CH2CHCH2OO(1)  2.260e+12     0.00        0.00
!     CH2CHCH2OO(1)=CHCHCH2OOH(2)         4.936e+06     1.55
26636.00
!     C2H2+CH2OOH=CHCHCH2OOH(2)     1.999e+10     0.00        6975.00
!     CH2CHCH2OO(1)=CH2cyCHCH2OO(3)       2.724e+10     0.48
29169.00
!     CH2CHO+CH2O=CH2cyCHCH2OO(3)   4.638e-01     3.42        77107.00

C2H2+CH2OOH(+m)=aC3H5+O2(+m)        1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (CH2CHCH2OO)
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  6.8401000e+00 -5.7440000e-02 -6.6822000e-02 /
CHEB /  2.2860000e+00  1.0725000e-01  1.0711000e-01 /
CHEB / -2.2391000e-01 -5.3757000e-02 -3.5887000e-02 /
CHEB / -1.3591000e-01 -1.1610000e-02 -1.7431000e-02 /
CHEB / -7.9271000e-02  1.3284000e-02  8.6346000e-03 /
! For the above reaction, deltaHrxn(T=298K) = -28.4 kcal/mol

aC3H5+O2(+m)=CH2CHO+CH2O(+m)        1.0E0 0.0 0.0     !NetReaction from
PDepNetwork #3 (CH2CHCH2OO)
TCHEB / 290.0 3000.0 /  PCHEB / 0.009869232667160128 98.69232667160128 /
CHEB / 5    3 /
CHEB /  4.5455000e+00 -2.3171000e-01 -1.2835000e-01 /
CHEB /  5.6096000e+00  3.2813000e-01  1.7712000e-01 /
CHEB /  1.8396000e-01 -8.8545000e-02 -4.0271000e-02 /
CHEB /  5.4771000e-02 -2.2215000e-02 -1.5959000e-02 /
CHEB /  2.1213000e-02  1.1223000e-02  4.3608000e-03 /
! For the above reaction, deltaHrxn(T=298K) = -64.2 kcal/mol

END
```

2. Transport Properties:

```
AR                0   136.500     3.330     0.000     0.000     0.000
C                 0    71.400     3.298     0.000     0.000     0.000 !
*
C2                1    97.530     3.621     0.000     1.760     4.000
C2O               1   232.400     3.828     0.000     0.000     1.000 !
*
CN2               1   232.400     3.828     0.000     0.000     1.000 !
OIS
C2H               1   209.000     4.100     0.000     0.000     2.500
C2H2              1   209.000     4.100     0.000     0.000     2.500
C2H2OH            2   224.700     4.162     0.000     0.000     1.000 !
*
C2H3              2   209.000     4.100     0.000     0.000     1.000 !
*
C2H4              2   280.800     3.971     0.000     0.000     1.500
C2H5              2   252.300     4.302     0.000     0.000     1.500
C2H6              2   252.300     4.302     0.000     0.000     1.500
C2N               1   232.400     3.828     0.000     0.000     1.000 !
OIS
C2N2              1   349.000     4.361     0.000     0.000     1.000 !
OIS
C3H2              2   209.000     4.100     0.000     0.000     1.000 !
*
C3H4              1   252.000     4.760     0.000     0.000     1.000
C3H6              2   266.800     4.982     0.000     0.000     1.000
C3H7              2   266.800     4.982     0.000     0.000     1.000
C4H6              2   357.000     5.180     0.000     0.000     1.000
I*C3H7            2   266.800     4.982     0.000     0.000     1.000
N*C3H7            2   266.800     4.982     0.000     0.000     1.000
C3H8              2   266.800     4.982     0.000     0.000     1.000
C4H               1   357.000     5.180     0.000     0.000     1.000
C4H2              1   357.000     5.180     0.000     0.000     1.000
C4H2OH            2   224.700     4.162     0.000     0.000     1.000 !
*
C4H8              2   357.000     5.176     0.000     0.000     1.000
C4H9              2   357.000     5.176     0.000     0.000     1.000
I*C4H9            2   357.000     5.176     0.000     0.000     1.000
C5H2              1   357.000     5.180     0.000     0.000     1.000
C5H3              1   357.000     5.180     0.000     0.000     1.000
C6H2              1   357.000     5.180     0.000     0.000     1.000
C6H5              2   412.300     5.349     0.000     0.000     1.000 !
JAM
C6H5O             2   450.000     5.500     0.000     0.000     1.000 !
JAM
C5H5OH            2   450.000     5.500     0.000     0.000     1.000 !
JAM
C6H6              2   412.300     5.349     0.000     0.000     1.000 !
SVE
C6H7              2   412.300     5.349     0.000     0.000     1.000 !
JAM
CH                1    80.000     2.750     0.000     0.000     0.000
CH2               1   144.000     3.800     0.000     0.000     0.000
CH2(S)            1   144.000     3.800     0.000     0.000     0.000
CH2*              1   144.000     3.800     0.000     0.000     0.000
```

```
CH2CHCCH          2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH2CHCCH2         2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH2CHCH2          2   260.000     4.850     0.000     0.000     1.000 !
JAM
CH2CHCHCH         2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH2CHCHCH2        2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH2CO             2   436.000     3.970     0.000     0.000     2.000
CH2O              2   498.000     3.590     0.000     0.000     2.000
CH2OH             2   417.000     3.690     1.700     0.000     2.000
CH3               1   144.000     3.800     0.000     0.000     0.000
CH3CC             2   252.000     4.760     0.000     0.000     1.000 !
JAM
CH3CCCH2          2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH3CCCH3          2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH3CCH2           2   260.000     4.850     0.000     0.000     1.000 !
JAM
CH3CHCH           2   260.000     4.850     0.000     0.000     1.000 !
JAM
CH3CH2CCH         2   357.000     5.180     0.000     0.000     1.000 !
JAM
CH3CHO            2   436.000     3.970     0.000     0.000     2.000
CH2CHO            2   436.000     3.970     0.000     0.000     2.000
CH3CO             2   436.000     3.970     0.000     0.000     2.000
CH3O              2   417.000     3.690     1.700     0.000     2.000
CH3OH             2   481.800     3.626     0.000     0.000     1.000 !
SVE
CH4               2   141.400     3.746     0.000     2.600    13.000
CH4O              2   417.000     3.690     1.700     0.000     2.000
CN                1    75.000     3.856     0.000     0.000     1.000 !
OIS
CNC               1   232.400     3.828     0.000     0.000     1.000 !
OIS
CNN               1   232.400     3.828     0.000     0.000     1.000 !
OIS
CO                1    98.100     3.650     0.000     1.950     1.800
CO2               1   244.000     3.763     0.000     2.650     2.100
H                 0   145.000     2.050     0.000     0.000     0.000
H2C4O             2   357.000     5.180     0.000     0.000     1.000 !
JAM
H2                1    38.000     2.920     0.000     0.790   280.000
H2CCCCH           2   357.000     5.180     0.000     0.000     1.000 !
JAM
H2CCCCH2          2   357.000     5.180     0.000     0.000     1.000 !
JAM
H2CCCH            2   252.000     4.760     0.000     0.000     1.000 !
JAM
H2CN              1   569.000     3.630     0.000     0.000     1.000 !
os/jm
H2NO              2   116.700     3.492     0.000     0.000     1.000 !
JAM
H2O               2   572.400     2.605     1.844     0.000     4.000
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```
H2O2              2   107.400     3.458     0.000     0.000     3.800
HC2N2             1   349.000     4.361     0.000     0.000     1.000 !
OIS
HCCHCCH           2   357.000     5.180     0.000     0.000     1.000 !
JAM
HCCO              2   150.000     2.500     0.000     0.000     1.000 !
*
HCNN              2   150.000     2.500     0.000     0.000     1.000 !
*
HCCOH             2   436.000     3.970     0.000     0.000     2.000
HCN               1   569.000     3.630     0.000     0.000     1.000 !
OIS
HCO               2   498.000     3.590     0.000     0.000     0.000
HE                0    10.200     2.576     0.000     0.000     0.000 !
*
HCNO              2   232.400     3.828     0.000     0.000     1.000 !
JAM
HOCN              2   232.400     3.828     0.000     0.000     1.000 !
JAM
HNCO              2   232.400     3.828     0.000     0.000     1.000 !
OIS
HNNO              2   232.400     3.828     0.000     0.000     1.000 !
*
HNO               2   116.700     3.492     0.000     0.000     1.000 !
*
HNOH              2   116.700     3.492     0.000     0.000     1.000 !
JAM
HO2               2   107.400     3.458     0.000     0.000     1.000 !
*
N                 0    71.400     3.298     0.000     0.000     0.000 !
*
N2                1    97.530     3.621     0.000     1.760     4.000
N2H2              2    71.400     3.798     0.000     0.000     1.000 !
*
N2H3              2   200.000     3.900     0.000     0.000     1.000 !
*
N2H4              2   205.000     4.230     0.000     4.260     1.500
N2O               1   232.400     3.828     0.000     0.000     1.000 !
*
NCN               1   232.400     3.828     0.000     0.000     1.000 !
OIS
NCO               1   232.400     3.828     0.000     0.000     1.000 !
OIS
NH                1    80.000     2.650     0.000     0.000     4.000
NH2               2    80.000     2.650     0.000     2.260     4.000
NH3               2   481.000     2.920     1.470     0.000    10.000
NNH               2    71.400     3.798     0.000     0.000     1.000 !
*
NO                1    97.530     3.621     0.000     1.760     4.000
NCNO              2   232.400     3.828     0.000     0.000     1.000 !
OIS
NO2               2   200.000     3.500     0.000     0.000     1.000 !
*
O                 0    80.000     2.750     0.000     0.000     0.000
O2                1   107.400     3.458     0.000     1.600     3.800
OH                1    80.000     2.750     0.000     0.000     0.000
!Previous transport properties are those reported in GRI-Mech 3.0
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!Next set of transport properties are those reported by Marinov for
Ethanol Oxidation
HCOH                2   498.000     3.590     0.000     0.000     1.000
HCOOH               2   436.000     3.970     0.000     0.000     2.000
C2H5OH              2   470.600     4.410     0.000     0.000     1.500 !
nmm
sC3H5               2   316.000     4.220     0.000     0.000     1.000
pC3H5               2   316.000     4.220     0.000     0.000     1.000
C2H5O-3             2   470.600     4.410     0.000     0.000     1.500 !
nmm
CH3CO               2   436.000     3.970     0.000     0.000     2.000
HOC2H4O2            2   470.600     4.410     0.000     0.000     1.500
!7/01 same as c2h5oh, wjp
HCOCHO              2   440.200     4.010     0.000     0.000     2.000 !
nmm
C2O                 1   232.400     3.828     0.000     0.000     1.000 !
*
C3H4O-enone         2   443.200     4.120     0.000     0.000     1.000 !
nmm
C3H3O-enone         2   443.200     4.120     0.000     0.000     1.000 !
nmm
C3H7-2              2   303.400     4.810     0.000     0.000     1.000 !
nmm
C3H5O-enal          2   424.600     4.820     0.000     0.000     1.000

!Next set of transport properties are estimated (using empirical
correlations
!     and a group contributions scheme) for current study of 1-butanol
C3H2                1   330.094     4.785     0.000     0.000     1.000
!MRH
pC3H3               2   330.321     4.806     0.000     0.000     1.000
!MRH
pC3H4               2   330.321     4.883     0.000     0.000     1.000
!MRH
aC3H4               2   330.094     4.939     0.000     0.000     1.000
!MRH
aC3H5               2   329.034     5.052     0.000     0.000     1.000
!MRH
C3H7-1              2   329.050     5.150     0.000     0.000     1.000
!MRH
C4H2                1   352.107     4.860     0.000     0.000     1.000
!MRH
iC4H3               2   349.960     5.031     0.000     0.000     1.000
!MRH
nC4H3               2   349.960     5.031     0.000     0.000     1.000
!MRH
C4H4                2   349.960     5.109     0.000     0.000     1.000
!MRH
C4H6-12             2   360.199     5.294     0.000     0.000     1.000
!MRH
C4H6-13             2   348.358     5.353     0.000     0.000     1.000
!MRH
C4H7-14             2   348.235     5.376     0.000     0.000     1.000
!MRH
C4H7-24             2   358.834     5.406     0.000     0.000     1.000
!MRH
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C4H8-1              2   348.235     5.451     0.000     0.000     1.000
!MRH
C4H9-1              2   348.199     5.474     0.000     0.000     1.000
!MRH
nC4H10              2   348.199     5.548     0.000     0.000     1.000
!MRH
C2H4O               2   384.335     4.927     0.000     0.000     1.000
!MRH
C2H5O-1             2   384.316     4.952     0.000     0.000     1.000
!MRH
C2H5O-2             2   384.316     4.952     0.000     0.000     1.000
!MRH
C3H4O               2   376.994     5.183     0.000     0.000     1.000
!MRH
C3H5O-enol2         2   411.992     5.184     0.000     0.000     1.000
!MRH
C3H5OJ(8)           2   376.679     5.206     0.000     0.000     1.000
!MRH
C3H5OJ(12)          2   376.679     5.206     0.000     0.000     1.000
!MRH
C3H5OJ(13)          2   376.679     5.206     0.000     0.000     1.000
!MRH
C3H6O-enol2         2   402.148     5.250     0.000     0.000     1.000
!MRH
C3H6O               2   376.679     5.285     0.000     0.000     1.000
!MRH
C3H7O-N1            2   402.151     5.275     0.000     0.000     1.000
!MRH
C4H9O-1             2   419.712     5.596     0.000     0.000     1.000
!MRH
C4H9O-2             2   419.712     5.596     0.000     0.000     1.000
!MRH
C4H9O-3             2   419.712     5.596     0.000     0.000     1.000
!MRH
C4H9O-4             2   419.712     5.596     0.000     0.000     1.000
!MRH
C4H9O-5             2   419.712     5.596     0.000     0.000     1.000
!MRH
nC4H10O             2   419.712     5.676     0.000     0.000     1.000
!MRH
C4H8-2              2   358.834     5.482     0.000     0.000     1.000
!MRH
C4H9-2              2   348.199     5.474     0.000     0.000     1.000
!MRH
C4H7OJ(8)           2   394.626     5.526     0.000     0.000     1.000
!MRH
C4H7OJ(12)          2   394.626     5.526     0.000     0.000     1.000
!MRH
C4H7OJ(13)          2   394.626     5.526     0.000     0.000     1.000
!MRH
C4H7OJ(16)          2   394.626     5.526     0.000     0.000     1.000
!MRH
nC4H8O              2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H8O-enol          2   429.306     5.587     0.000     0.000     1.000
!MRH
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C4H8O-enol3         2   419.669     5.570     0.000     0.000     1.000
!MRH
C4H6-1              2   349.620     5.208     0.000     0.000     1.000
!MRH
C4H7-12             2   348.235     5.376     0.000     0.000     1.000
!MRH
C4H7-11             2   348.235     5.376     0.000     0.000     1.000
!MRH
C4H7O-13            2   419.669     5.489     0.000     0.000     1.000
!MRH
C4H8O-enol2         2   429.306     5.587     0.000     0.000     1.000
!MRH
C2H3O-1             2   384.335     4.844     0.000     0.000     1.000
!MRH
C2H3O-2             2   384.335     4.844     0.000     0.000     1.000
!MRH
nC4H5               2   348.358     5.278     0.000     0.000     1.000
!MRH
C4H5-113            2   349.620     5.131     0.000     0.000     1.000
!MRH
iC4H5               2   348.358     5.278     0.000     0.000     1.000
!MRH
C3H6O-enol          2   411.992     5.266     0.000     0.000     1.000
!MRH
C4H4-123            2   361.817     5.102     0.000     0.000     1.000
!MRH
C4H6-2              2   376.099     5.307     0.000     0.000     1.000
!MRH
C4H7-22             2   358.834     5.406     0.000     0.000     1.000
!MRH
C6H10               2   385.191     5.993     0.000     0.000     1.000
!MRH
C6H9_1_2_5          2   385.191     5.918     0.000     0.000     1.000
!MRH
C6H9_CYC_1_3        2   436.440     5.695     0.000     0.000     1.000
!MRH
C6H8_CYC_1_4        2   437.544     5.689     0.000     0.000     1.000
!MRH
C6H7_CYC_1_2        2   437.544     5.607     0.000     0.000     1.000
!MRH
C6H10_CYC           2   436.440     5.776     0.000     0.000     1.000
!MRH
C7H9                2   459.165     5.985     0.000     0.000     1.000
!MRH
C8H8                2   477.487     6.192     0.000     0.000     1.000
!MRH
C8H9                2   476.287     6.212     0.000     0.000     1.000
!MRH
C7H8                2   460.269     5.979     0.000     0.000     1.000
!MRH
C3H7O2              2   420.058     5.396     0.000     0.000     1.000
!MRH
CH2CH2CH2OOH        2   420.058     5.396     0.000     0.000     1.000
!MRH
aC3H5O2             2   420.040     5.287     0.000     0.000     1.000
!MRH
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nSPC(301)          2   507.337     5.736     0.000     0.000     1.000
!MRH
nSPC(351)          2   507.337     5.736     0.000     0.000     1.000
!MRH
nSPC(385)          2   482.430     5.774     0.000     0.000     1.000
!MRH
nSPC(447)          2   465.344     5.575     0.000     0.000     1.000
!MRH
nSPC(543)          2   446.256     5.050     0.000     0.000     1.000
!MRH
nSPC(801)          2   437.019     5.156     0.000     0.000     1.000
!MRH
nSPC(879)          2   520.947     5.251     0.000     0.000     1.000
!MRH
nSPC(1064)         2   451.626     5.139     0.000     0.000     1.000
!MRH
nSPC(102)          2   384.692     4.665     0.000     0.000     1.000
!MRH
C5H10_1            2   366.871     5.772     0.000     0.000     1.000
!MRH
C5H9_1_4           2   366.871     5.697     0.000     0.000     1.000
!MRH
C5H8_CYC_1         2   409.083     5.475     0.000     0.000     1.000
!MRH
C5H9_CYC           2   408.079     5.481     0.000     0.000     1.000
!MRH
C5H7_CYC_1_2       2   409.083     5.394     0.000     0.000     1.000
!MRH

!Next set of transport properties are those reported by S. Sharma et al.
!     in their study on hexadiene isomers
!NOTE: Changed some of the structure indicator values from 1 to 2
FULVENE            2   395.000     6.000     0.000     0.000     1.000
benzene            2   380.000     5.250     0.000     0.000     1.000!
(EST)
C6H4               2   395.000     6.000     0.000     0.000     1.000
C5H5               2   357.000     5.180     0.000     0.000     1.000
C6H5OH             2   450.000     5.500     0.000     0.000     1.000 !
nmm
cyC5H6             2   357.000     5.180     0.000     0.000     1.000
C5H5CH3_1          2   395.000     6.000     0.000     0.000     1.000
C5H5CH3_2          2   395.000     6.000     0.000     0.000     1.000
C5H5CH3_3          2   395.000     6.000     0.000     0.000     1.000
C8H6               2   495.300     5.680     0.000     0.000     1.000 !
nmm
C6H5CH3            2   495.300     5.680     0.430     12.30     1.000 !
nmm
C6H5CH2            2   495.300     5.680     0.000     0.000     1.000 !
nmm
C6H5C2H3           2   546.200     6.000     0.130     15.00     1.000 !
nmm
C6H5CCH2           2   546.200     6.000     0.000     0.000     1.000
C5H4CH3            2   395.000     6.000     0.000     0.000     1.000
C5H5CH2-1          2   395.000     6.000     0.000     0.000     1.000
C5H5CH2-2          2   395.000     6.000     0.000     0.000     1.000
C5H5CH2-3          2   395.000     6.000     0.000     0.000     1.000
ME2CYBE            2   395.000     6.000     0.000     0.000     1.000
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c5h4chchch2        2   380.000     5.250     0.000     0.000     1.000
cyC6H7             2   412.300     5.349     0.000     0.000     1.000
C#CCCC#C           2   395.000     6.000     0.000     0.000     1.000
C*C*CC*C*C         2   395.000     6.000     0.000     0.000     1.000
CH3CCCH2           2   357.000     5.180     0.000     0.000     1.000

!Next set of transport properties are estimated (using empirical
correlations
!     and a group contributions scheme) for current study of 2-butanol
sBuOH              2   422.223     5.667     0.000     0.000     1.000
!MRH
CH3CH[OH]CH2       2   404.746     5.266     0.000     0.000     1.000
!MRH
C2H5CHOH           2   402.151     5.275     0.000     0.000     1.000
!MRH
CH3C[OH]C2H5       2   422.223     5.587     0.000     0.000     1.000
!MRH
MEK                2   402.939     5.671     0.000     0.000     1.000
!MRH
CH3CH[OH]CHCH3     2   422.223     5.587     0.000     0.000     1.000
!MRH
CH3CH[OH]CH2CH2    2   422.223     5.587     0.000     0.000     1.000
!MRH
sC4H8O             2   422.279     5.562     0.000     0.000     1.000
!MRH
CH3CH[O]C2H5       2   422.223     5.587     0.000     0.000     1.000
!MRH
HOCHC2H5           2   402.151     5.275     0.000     0.000     1.000
!MRH
H2CCCH3[OH]        2   404.630     5.248     0.000     0.000     1.000
!MRH
acetone            2   385.191     5.352     0.000     0.000     1.000
!MRH
CH2CH[OH]C2H5      2   422.223     5.587     0.000     0.000     1.000
!MRH
CH3CH-O-CH3        2   348.599     5.291     0.000     0.000     1.000
!MRH
CH3C[OH]CH3        2   348.371     5.242     0.000     0.000     1.000
!MRH
C2H5CHCHCH2        2   366.871     5.697     0.000     0.000     1.000
!MRH
CH2C[OH]CH2        2   404.630     5.165     0.000     0.000     1.000
!MRH
CH3-O-C(CH3)2      2   370.007     5.607     0.000     0.000     1.000
!MRH
CH2C[O]CH3         2   385.191     5.272     0.000     0.000     1.000
!MRH
cH2C[O]C2H5        2   402.939     5.592     0.000     0.000     1.000
!MRH
CH3C[O]cHCH3       2   402.939     5.592     0.000     0.000     1.000
!MRH
CH3C[O]CH2cH2      2   402.939     5.592     0.000     0.000     1.000
!MRH
MEKenol2           2   422.076     5.568     0.000     0.000     1.000
!MRH
CH2C[OH]cHCH3      2   422.076     5.487     0.000     0.000     1.000
!MRH
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CH2C[OH]CH2cH2      2   422.076     5.487     0.000     0.000     1.000
!MRH
cHC[OH]C2H5         2   422.076     5.487     0.000     0.000     1.000
!MRH
MEKenol             2   431.804     5.585     0.000     0.000     1.000
!MRH
CH3CHcOH            2   411.992     5.184     0.000     0.000     1.000
!MRH
CH3C[OH]cH          2   404.630     5.165     0.000     0.000     1.000
!MRH
CH3C[OH]cCH3        2   431.804     5.503     0.000     0.000     1.000
!MRH
CH3C[OH]CHcH2       2   431.804     5.503     0.000     0.000     1.000
!MRH
cH2CH[OH]C2H3       2   422.279     5.480     0.000     0.000     1.000
!MRH
CH3CH[OH]cCH2       2   422.279     5.480     0.000     0.000     1.000
!MRH
CH3CH[OH]CHcH       2   422.279     5.480     0.000     0.000     1.000
!MRH
CH3CH[o]C2H3        2   422.279     5.480     0.000     0.000     1.000
!MRH
C4H6O(717)          2   380.111     5.446     0.000     0.000     1.000
!MRH
C4H7O_1_2           2   446.407     5.577     0.000     0.000     1.000
!MRH
CH3CHCHCHO          2   380.111     5.446     0.000     0.000     1.000
!MRH
CHCHCHO             2   443.200     4.120     0.000     0.000     1.000 !
nmm
CH3CCHCHO           2   405.314     5.446     0.000     0.000     1.000
!MRH
CH3CHCHCO           2   405.314     5.446     0.000     0.000     1.000
!MRH
C4H7O-14            2   419.669     5.489     0.000     0.000     1.000
!MRH

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!
! New work for sec- and tert-butanol paper:
!
!    "Accurate Reaction Networks for Alternative Fuels: Butanol Isomers"
!
!    K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
!
!    To be submitted to Industrial & Engineering Chemical Research
!
!       for the ISCRE-21 conference
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!

tBuOH               2   425.369     5.654     0.000     0.000     1.000
!MRH
iC4H8               2   350.926     5.453     0.000     0.000     1.000
!MRH
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HOC[CH2][CH3]2     2   425.369     5.573     0.000     0.000     1.000
!MRH
OC[CH3]3           2   425.369     5.573     0.000     0.000     1.000
!MRH
iC4H7              2   350.926     5.378     0.000     0.000     1.000
!MRH
HCC[CH3]2          2   350.926     5.378     0.000     0.000     1.000
!MRH
iC4H10             2   351.020     5.545     0.000     0.000     1.000
!MRH
iC4H9              2   351.020     5.470     0.000     0.000     1.000
!MRH
tC4H9              2   351.020     5.470     0.000     0.000     1.000
!MRH
sSPC(116)          2   509.380     5.721     0.000     0.000     1.000
!MRH
sSPC(46)           2   439.859     5.599     0.000     0.000     1.000
!MRH
sSPC(56)           2   446.786     5.623     0.000     0.000     1.000
!MRH
sSPC(752)          2   489.920     5.747     0.000     0.000     1.000
!MRH
sSPC(332)          2   507.337     5.736     0.000     0.000     1.000
!MRH
sSPC(1013)         2   507.337     5.736     0.000     0.000     1.000
!MRH
sSPC(1072)         2   487.377     5.844     0.000     0.000     1.000
!MRH
sSPC(1151)         2   470.344     5.646     0.000     0.000     1.000
!MRH
sSPC(1356)         2   470.732     5.435     0.000     0.000     1.000
!MRH
sSPC(1697)         2   384.692     4.749     0.000     0.000     1.000
!MRH
sSPC(1735)         2   384.692     4.833     0.000     0.000     1.000
!MRH
sSPC(1909)         2   436.658     4.910     0.000     0.000     1.000
!MRH
sSPC(3071)         2   429.181     4.722     0.000     0.000     1.000
!MRH
sSPC(3121)         2   429.181     4.811     0.000     0.000     1.000
!MRH
sSPC(2810)         2   342.153     4.682     0.000     0.000     1.000
!MRH
sSPC(1474)         2   470.732     5.522     0.000     0.000     1.000
!MRH
sSPC(1590)         2   453.576     5.323     0.000     0.000     1.000
!MRH

tSPC(54)           2   439.663     5.606     0.000     0.000     1.000
!MRH
tSPC(77)           2   439.663     5.606     0.000     0.000     1.000
!MRH
tSPC(122)          2   523.993     5.737     0.000     0.000     1.000
!MRH
tSPC(157)          2   532.663     5.740     0.000     0.000     1.000
!MRH
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tSPC(213)          2   482.318     5.669     0.000     0.000     1.000
!MRH
tSPC(97)           2   509.511     5.714     0.000     0.000     1.000
!MRH
tSPC(439)          2   509.511     5.714     0.000     0.000     1.000
!MRH
tSPC(343)          2   465.284     5.471     0.000     0.000     1.000
!MRH
tSPC(346)          2   376.994     5.103     0.000     0.000     1.000
!MRH
tSPC(878)          2   465.694     5.258     0.000     0.000     1.000
!MRH
H2CCCO             2   324.173     4.451     0.000     0.000     1.000
!MRH
tSPC(1286)         2   454.139     5.368     0.000     0.000     1.000
!MRH
tSPC(1416)         2   454.139     5.453     0.000     0.000     1.000
!MRH
tSPC(1553)         2   469.347     5.449     0.000     0.000     1.000
!MRH
C8H14              2   403.432     6.536     0.000     0.000     1.000
!MRH
tSPC(3683)         2   470.732     5.435     0.000     0.000     1.000
!MRH
C4H8O2(62)         2   439.663     5.688     0.000     0.000     1.000
!MRH
C4H7OJ(79)         2   422.076     5.487     0.000     0.000     1.000
!MRH
tSPC(110)          2   397.587     5.441     0.000     0.000     1.000
!MRH
C4H6O(105)         2   409.324     5.357     0.000     0.000     1.000
!MRH

C4H6O(167)         2   397.738     5.504     0.000     0.000     1.000
!MRH
SPC(875)           2   430.538     5.363     0.000     0.000     1.000
!MRH
SPC(194)           2   397.738     5.424     0.000     0.000     1.000
!MRH
SPC(1454)          2   511.012     6.672     0.000     0.000     1.000
!MRH
SPC(913)           2   430.538     5.279     0.000     0.000     1.000
!MRH
SPC(1787)          2   416.927     4.786     0.000     0.000     1.000
!MRH

C5H10_iso          2   369.515     5.774     0.000     0.000     1.000
!MRH
C5H9J(5)           2   369.515     5.699     0.000     0.000     1.000
!MRH
C5H9J(7)           2   369.515     5.699     0.000     0.000     1.000
!MRH
C5H9J(8)           2   369.515     5.699     0.000     0.000     1.000
!MRH
C5H9J(9)           2   369.515     5.699     0.000     0.000     1.000
!MRH
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C5H11J(10)          2   369.584     5.791     0.000     0.000     1.000
!MRH
C5H11J(11)          2   369.584     5.791     0.000     0.000     1.000
!MRH

C5H8(95)            2   369.756     5.677     0.000     0.000     1.000
!MRH
SPC(482)            2   438.094     6.476     0.000     0.000     1.000
!MRH
SPC(483)            2   434.128     6.482     0.000     0.000     1.000
!MRH
C5H7J(504)          2   378.586     5.538     0.000     0.000     1.000
!MRH
SPC(493)            2   438.803     6.378     0.000     0.000     1.000
!MRH
SPC(494)            2   437.495     6.386     0.000     0.000     1.000
!MRH
SPC(495)            2   444.537     6.416     0.000     0.000     1.000
!MRH
SPC(496)            2   434.619     6.384     0.000     0.000     1.000
!MRH
SPC(498)            2   417.029     6.168     0.000     0.000     1.000
!MRH
SPC(499)            2   421.147     6.162     0.000     0.000     1.000
!MRH
C6H7J(511)          2   399.882     5.759     0.000     0.000     1.000
!MRH
C6H7J(512)          2   396.940     5.757     0.000     0.000     1.000
!MRH
C6H7J(505)          2   399.882     5.759     0.000     0.000     1.000
!MRH
C6H7J(506)          2   407.519     5.783     0.000     0.000     1.000
!MRH
C8H13J(41)          2   435.559     6.580     0.000     0.000     1.000
!MRH
C8H15J(44)          2   425.511     6.644     0.000     0.000     1.000
!MRH
SPC(425)            2   490.788     7.313     0.000     0.000     1.000
!MRH
SPC(426)            2   487.009     7.320     0.000     0.000     1.000
!MRH
C7H10(454)          2   407.355     6.070     0.000     0.000     1.000
!MRH

!Updated by MRH 7/JUN/2010
iBuOH               2   422.223     5.667     0.000     0.000     1.000
!MRH
C3H7O-N2            2   402.151     5.275     0.000     0.000     1.000
!MRH
C4H9Oi1             2   422.223     5.587     0.000     0.000     1.000
!MRH
C4H9Oi2             2   422.223     5.587     0.000     0.000     1.000
!MRH
C4H9Oi3             2   422.223     5.587     0.000     0.000     1.000
!MRH
C4H9Oi4             2   422.223     5.587     0.000     0.000     1.000
!MRH
```

```
C4H8O-i2           2   431.804     5.585     0.000     0.000     1.000
!MRH
C4H8O-i3           2   397.587     5.599     0.000     0.000     1.000
!MRH
C4H8O-i1           2   422.076     5.568     0.000     0.000     1.000
!MRH

!Updated by MRH 9/JUL/2010
C12H10             2   598.435     6.936     0.000     0.000     1.000
!MRH
biC5H5             2   529.095     6.568     0.000     0.000     1.000
!MRH
C5H4C5H5           2   529.095     6.484     0.000     0.000     1.000
!MRH
fulvalene          2   547.832     6.453     0.000     0.000     1.000
!MRH
C10H9              2   529.095     6.485     0.000     0.000     1.000
!MRH
C10H8              2   547.832     6.453     0.000     0.000     1.000
!MRH

!Updated by MRH 21/JUL/2010
iC4H7OJ(15)        2   422.076     5.487     0.000     0.000     1.000
!MRH
iC4H7OJ(17)        2   422.076     5.487     0.000     0.000     1.000
!MRH
iC4H7OJ(30)        2   431.804     5.503     0.000     0.000     1.000
!MRH
iC4H7OJ(48)        2   397.587     5.520     0.000     0.000     1.000
!MRH
iC4H7OJ(51)        2   397.587     5.520     0.000     0.000     1.000
!MRH
C3H3OH             2   413.194     5.058     0.000     0.000     1.000
!MRH
C4H6Oi-12          2   402.720     5.487     0.000     0.000     1.000
!MRH
C4H6Oi-13          2   397.738     5.504     0.000     0.000     1.000
!MRH
iC4H5OJ(14)        2   397.738     5.424     0.000     0.000     1.000
!MRH
iC4H5OJ(15)        2   397.738     5.424     0.000     0.000     1.000
!MRH
C3H3OJ(9)          2   413.194     4.973     0.000     0.000     1.000
!MRH
HCCCHO             2   379.037     4.925     0.000     0.000     1.000
!MRH
C3H3OJ             2   323.310     4.570     0.000     0.000     1.000
!MRH
C3H5OJ             2   402.148     5.168     0.000     0.000     1.000
!MRH
C3H5OJ(17)         2   411.992     5.184     0.000     0.000     1.000
!MRH
nC3H7OH            2   402.151     5.356     0.000     0.000     1.000
!MRH

!26AUG2010
```

```
C4H7OJ(9)          2   446.407     5.577     0.000     0.000     1.000
!MRH
C4H9O2J(52)        2   446.407     5.577     0.000     0.000     1.000
!MRH
C4H9O2J(53)        2   446.407     5.577     0.000     0.000     1.000
!MRH
C4H9O2J(54)        2   446.407     5.577     0.000     0.000     1.000
!MRH
C4H9O2J(55)        2   446.407     5.577     0.000     0.000     1.000
!MRH

C4H7OJ(118)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(119)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(158)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(159)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(160)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(204)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(205)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7OJ(207)        2   394.626     5.605     0.000     0.000     1.000
!MRH

CH2CHCHCHOH        2   394.626     5.605     0.000     0.000     1.000
!MRH
CH2CHCCHOH         2   394.626     5.605     0.000     0.000     1.000
!MRH
CHCHCHCHOH         2   394.626     5.605     0.000     0.000     1.000
!MRH
CH2CHCHCOH         2   394.626     5.605     0.000     0.000     1.000
!MRH
CHCCHCHOH          2   394.626     5.605     0.000     0.000     1.000
!MRH
CHCCCHOH           2   394.626     5.605     0.000     0.000     1.000
!MRH

C4H5O3J(1)         2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5O3J(2)         2   394.626     5.605     0.000     0.000     1.000
!MRH
OCOOH              2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H6O3(21)         2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5O2J(12)        2   394.626     5.605     0.000     0.000     1.000
!MRH
CH2CHCHCHO         2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5O2J(13)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H6O3(3)          2   394.626     5.605     0.000     0.000     1.000
!MRH
```

```
C4H7O3J(1)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7O3J(2)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7O3J(3)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7O3J(4)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7O3J(5)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H7O3J(6)          2   394.626     5.605     0.000     0.000     1.000
!MRH
C3H5O2J(54)         2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5O3J(3)          2   394.626     5.605     0.000     0.000     1.000
!MRH
CH2CHCH2O           2   394.626     5.605     0.000     0.000     1.000
!MRH

C4H5O2J(100)        2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5O2J(101)        2   394.626     5.605     0.000     0.000     1.000
!MRH
OCH2CH2CH3          2   394.626     5.605     0.000     0.000     1.000
!MRH
CH2OOH              2   394.626     5.605     0.000     0.000     1.000
!MRH
HOCHOOH             2   394.626     5.605     0.000     0.000     1.000
!MRH
C4H5-114            2   349.620     5.131     0.000     0.000     1.000
!MRH
C5H9_2_4            2   366.871     5.697     0.000     0.000     1.000
!MRH
CHCHCH2OH           2   402.148     5.250     0.000     0.000     1.000
!MRH

CCCC(OO)OH          2   402.148     5.250     0.000     0.000     1.000
!MRH
CcCC(OOH)OH         2   402.148     5.250     0.000     0.000     1.000
!MRH

HOOCH2CO            2   275.049     5.428     0.000     0.000     1.000 !
LJ parameters estimated by RMG: Tc= 579.553K Pc=  66.206bar Vc=
201.500cm3/mol Tb= 408.420K   (Alcohol, Ether, CsH2R2,
Aldehyde_Ccentered, Aldehyde_Ocentered)
```

3. Dictionary:

```
H2
1 H 0 {2,S}
2 H 0 {1,S}

CO2
1 C 0 {2,D} {3,D}
2 O 0 {1,D}
3 O 0 {1,D}

CO
1 C 2T {2,D}
2 O 0 {1,D}

CH4
1 C 0

C2H4
1 C 0 {2,D}
2 C 0 {1,D}

C2H2
1 C 0 {2,T}
2 C 0 {1,T}

C2H6
1 C 0 {2,S}
2 C 0 {1,S}

C3H6
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S}

C3H8
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S}

aC3H4
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 C 0 {2,D}

pC3H4
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S}

CH3OH
1 C 0 {2,S}
2 O 0 {1,S}

C4H8-1
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
```

```
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C4H6-13
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}

nC4H10
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

// N2 is commented out because RMG cannot parse "N"
//N2
//1 N 0 {2,T}
//2 N 0 {1,T}

C2H5OH
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 O 0 {2,S}

benzene
1 C 0 {6,S} {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}

nC4H10O
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C2H3
1 C 1 {2,D}
2 C 0 {1,D}

CH2CO
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 O 0 {2,D}

C2H4O
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 O 0 {2,S}

CH3CHO
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
```

```
3 O 0 {2,D}

H2O
1 O 0

nC4H8O
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

C4H7OJ(8)
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S} {5,D}
5 O 0 {4,D}

C4H7OJ(12)
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

C4H7OJ(13)
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

C4H7OJ(16)
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

CH2CHO
1 C 1 {2,S}
2 C 0 {1,S} {3,D}
3 O 0 {2,D}

C3H6O-enol2
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

C3H5O-enol2
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 O 0 {3,S}
```

```
CH2O
1 C 0 {2,D}
2 O 0 {1,D}

C4H8O-enol
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

C4H8O-enol2
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H8O-enol3
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H9O-1
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H9O-2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H9O-3
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H9O-4
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S} {5,S}
5 O 0 {4,S}

C4H9O-5
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
```

```
4 C 0 {3,S} {5,S}
5 O 1 {4,S}

C3H7O-N1
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

C3H5OJ(8)
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 1 {2,S} {4,D}
4 O 0 {3,D}

C3H5OJ(12)
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

C3H5OJ(13)
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

C3H6O
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

C2H5
1 C 1 {2,S}
2 C 0 {1,S}

H
1 H 1

O
1 O 2T

O2
1 O 1 {2,S}
2 O 1 {1,S}

OH
1 O 1

HO2
1 O 1 {2,S}
2 O 0 {1,S}

H2O2
1 O 0 {2,S}
2 O 0 {1,S}
```

```
C
1 C 4

CH
1 C 3

CH2
1 C 2T

CH2(S)
1 C 2S

CH3
1 C 1

HCO
1 C 1 {2,D}
2 O 0 {1,D}

CH2OH
1 C 1 {2,S}
2 O 0 {1,S}

CH3O
1 C 0 {2,S}
2 O 1 {1,S}

C2H
1 C 1 {2,T}
2 C 0 {1,T}

HCCO
1 C 1 {2,D}
2 C 0 {1,D} {3,D}
3 O 0 {2,D}

HCCOH
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 O 0 {2,S}

// AR is commented out because RMG cannot parse "AR"
//1 AR 0

C2O
1 C 2 {2,D}
2 C 0 {1,D} {3,D}
3 O 0 {2,D}

HOC2H4O2
1 O 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 1 {4,S}
```

```
C3H2
1 C 1 {2,D}
2 C 0 {1,D} {3,D}
3 C 1 {2,D}

pC3H3
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 1 {2,S}

aC3H5
1 C 1 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D}

pC3H5
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 1 {2,D}

sC3H5
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D}

C3H7-1
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S}

C3H7-2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S}

C2H5O-1
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 O 0 {2,S}

C2H5O-2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 O 0 {2,S}

C2H5O-3
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 O 1 {2,S}

C3H4O-enone
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,D}
4 O 0 {3,D}

C3H4O
```

```
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

C4H7O-13
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}

C4H2
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,T}
4 C 0 {3,T}

iC4H3
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 1 {2,S} {4,D}
4 C 0 {3,D}

nC4H3
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,D}
4 C 1 {3,D}

C4H4
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}

C4H5-113
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S}

nC4H5
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 1 {3,D}

iC4H5
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,D}
4 C 0 {3,D}

C4H6-1
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
```

```
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C4H6-12
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S}

C4H7-14
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S}

C4H7-11
1 C 1 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C4H7-12
1 C 0 {2,D}
2 C 1 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C4H7-24
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S}

C4H9-1
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C4H9-2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

C2H3O-1
1 C 1 {2,D}
2 C 0 {1,D} {3,S}
3 O 0 {2,S}

C2H3O-2
1 C 0 {2,D}
2 C 1 {1,D} {3,S}
3 O 0 {2,S}

C6H4
1 C 0 {6,T} {2,S}
```

```
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,T}

C6H5
1 C 1 {6,D} {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,D}

C4H6-2
1 C 0 {2,S}
2 C 0 {1,S} {3,T}
3 C 0 {2,T} {4,S}
4 C 0 {3,S}

C4H7-22
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S}

CH3CO
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 O 0 {2,D}

C6H10
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D}

C6H9_1_2_5
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D}

C6H9_CYC_1_3
1 C 0 {2,D} {6,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S} {5,S}
5 C 0 {4,S} {6,S}
6 C 0 {5,S} {1,S}

C6H8_CYC_1_4
1 C 0 {2,D} {6,S}
```

```
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,S}

C6H7_CYC_1_2
1 C 0 {2,D} {6,S}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,S}

C6H10_CYC
1 C 0 {2,D} {6,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {6,S}
6 C 0 {5,S} {1,S}

C7H9
1 C 1 {6,S} {2,S} {7,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,S}
7 C 0 {1,S}

C8H8
1 C 0 {6,D} {2,S} {7,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,D}
7 C 0 {1,S} {8,D}
8 C 0 {7,D}

C8H9
1 C 0 {6,D} {2,S} {7,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
6 C 0 {5,S} {1,D}
7 C 0 {1,S} {8,S}
8 C 1 {7,S}

C7H8
1 C 0 {6,D} {2,S} {7,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,S}
```

```
6 C 0 {5,S} {1,D}
7 C 0 {1,S}

C3H7O2
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 1 {4,S}

CH2CH2CH2OOH
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 0 {4,S}

aC3H5O2
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 1 {4,S}

nSPC(301)
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {6,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}
6 O 0 {2,S} {7,S}
7 O 1 {6,S}

nSPC(351)
1  C 0 {2,S}
2  C 0 {1,S} {3,S} {6,S}
3  C 0 {2,S} {4,S}
4  C 1 {3,S} {5,S}
5  O 0 {4,S}
6  O 0 {2,S} {7,S}
7  O 0 {6,S}

nSPC(385)
1  C 0 {2,S}
2  C 0 {1,S} {3,S} {6,S}
3  C 0 {2,S} {4,S}
4  C 0 {3,S} {5,D}
5  O 0 {4,D}
6  O 0 {2,S} {7,S}
7  O 0 {6,S}

nSPC(447)
1  C 0 {2,S}
2  C 0 {1,S} {3,S} {6,S}
3  C 0 {2,S} {4,S}
4  C 0 {3,S} {5,D}
5  O 0 {4,D}
```

```
6  O 1 {2,S}

nSPC(543)
1 O 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 1 {4,S}

nSPC(801)
1 C 1 {2,S}
2 C 0 {1,S} {3,D} {4,S}
3 O 0 {2,D}
4 O 0 {2,S} {5,S}
5 O 0 {4,S}

nSPC(879)
1 C 0 {2,S} {6,S}
2 C 0 {1,S} {3,D} {4,S}
3 O 0 {2,D}
4 O 0 {2,S} {5,S}
5 O 0 {4,S}
6 O 0 {1,S} {7,S}
7 O 1 {6,S}

nSPC(1064)
1 O 1 {2,S}
2 O 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 1 {4,S}

nSPC(102)
1 O 1 {2,S}
2 O 0 {1,S} {3,S}
3 C 1 {2,S}

C4H8-2
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S}

C3H3O-enone
1 C 1 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,D}
4 O 0 {3,D}

FULVENE
1 C 0 {2,S} {5,S} {6,D}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {1,S}
6 C 0 {1,D}
```

```
C6H5O
1 C 0 {2,D} {6,S} {7,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}
7 O 1 {1,S}

C5H5
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 1 {4,S} {1,S}

C6H5OH
1 C 0 {2,D} {6,S} {7,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}
7 O 0 {1,S}

cyC5H6
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {1,S}

C5H5CH3_1
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {1,S} {6,S}
6 C 0 {5,S}

C5H5CH3_2
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S} {6,S}
5 C 0 {4,S} {1,S}
6 C 0 {4,S}

C5H5CH3_3
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D} {6,S}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {1,S}
6 C 0 {3,S}
```

```
C8H6
1 C 0 {2,D} {6,S} {7,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}
7 C 0 {1,S} {8,T}
8 C 0 {7,T}

C6H5CH2
1 C 0 {2,D} {6,S} {7,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}
7 C 1 {1,S}

C6H5CCH2
1 C 0 {2,D} {6,S} {7,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {6,D}
6 C 0 {5,D} {1,S}
7 C 1 {1,S} {8,D}
8 C 0 {7,D}

C5H4CH3
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 1 {4,S} {1,S} {6,S}
6 C 0 {5,S}

C5H5CH2-1
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {1,S} {6,S}
6 C 1 {5,S}

C5H5CH2-2
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S} {6,S}
5 C 0 {4,S} {1,S}
6 C 1 {4,S}

C5H5CH2-3
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D} {6,S}
```

```
4 C 0 {3,D} {5,S}
5 C 0 {4,S} {1,S}
6 C 1 {3,S}

ME2CYBE
1 C 0 {2,S} {4,S} {5,D}
2 C 0 {1,S} {3,S} {6,D}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {1,S}
5 C 0 {1,D}
6 C 0 {2,D}

c5h4chchch2
1 C 0 {2,S} {5,S} {6,D}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {1,S}
6 C 0 {1,D} {7,S}
7 C 0 {6,S} {8,D}
8 C 0 {7,D}

C#CCCC#C
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {6,T}
6 C 0 {5,T}

C*C*CC*C*C
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D} {6,D}
6 C 0 {5,D}

CH3CCCH2
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,D}
4 C 0 {3,D}

C4H4-123
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 C 0 {2,D} {4,D}
4 C 0 {3,D}

C5H10_1
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S}
```

```
C5H9_1_4
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 1 {4,S}

C5H8_CYC_1
1 C 0 {5,S} {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {1,S}

C5H9_CYC
1 C 1 {5,S} {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {1,S}

C5H7_CYC_1_2
1 C 0 {5,S} {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {1,S}

C4H7O_1_2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

sBuOH
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3C[OH]C2H5
1 C 0 {2,S}
2 C 1 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3CH[OH]CHCH3
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3CH[O]C2H5
```

```
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 1 {2,S}

CH2CH[OH]C2H5
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3CH[OH]CH2CH2
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S}
5 O 0 {2,S}

CH3CH[OH]CH2
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {4,S}
3 C 1 {2,S}
4 O 0 {2,S}

HOCHC2H5
1 O 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}

H2CCCH3[OH]
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 0 {2,S}
4 O 0 {2,S}

CH3CH-O-CH3
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 O 0 {2,S} {4,S}
4 C 0 {3,S}

CH3C[OH]CH3
1 C 0 {2,S}
2 C 1 {1,S} {3,S} {4,S}
3 C 0 {2,S}
4 O 0 {2,S}

acetone
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {4,D}
3 C 0 {2,S}
4 O 0 {2,D}

C2H5CHCHCH2
```

```
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 C 0 {4,D}

CH2C[OH]CH2
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 1 {2,S}
4 O 0 {2,S}

CH2C[O]CH3
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 0 {2,S}
4 O 1 {2,S}

CH3-O-C(CH3)2
1 C 0 {2,S}
2 O 0 {1,S} {3,S}
3 C 1 {2,S} {4,S} {5,S}
4 C 0 {3,S}
5 C 0 {3,S}

C3H6O-enol
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 O 0 {3,S}

MEK
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,D}

sC4H8O
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}
5 O 0 {2,S}

C4H6O(717)
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}
5 O 0 {2,D}

cH2C[O]C2H5
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
```

```
5 O 0 {2,D}

CH3C[O]cHCH3
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 1 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,D}

CH3C[O]CH2cH2
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 0 {2,S} {4,S}
4 C 1 {3,S}
5 O 0 {2,D}

MEKenol2
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH2C[OH]cHCH3
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH2C[OH]CH2cH2
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S}
5 O 0 {2,S}

cHC[OH]C2H5
1 C 1 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

MEKenol
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {5,S}
3 C 0 {2,D} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3CHcOH
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 1 {2,D} {4,S}
4 O 0 {3,S}
```

```
CH3C[OH]cH
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {4,S}
3 C 1 {2,D}
4 O 0 {2,S}

CH3C[OH]cCH3
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {5,S}
3 C 1 {2,D} {4,S}
4 C 0 {3,S}
5 O 0 {2,S}

CH3C[OH]CHcH2
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {5,S}
3 C 0 {2,D} {4,S}
4 C 1 {3,S}
5 O 0 {2,S}

cH2CH[OH]C2H3
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}
5 O 0 {2,S}

CH3CH[OH]cCH2
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 1 {2,S} {4,D}
4 C 0 {3,D}
5 O 0 {2,S}

CH3CH[OH]CHcH
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 C 1 {3,D}
5 O 0 {2,S}

CH3CH[o]C2H3
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D}
5 O 1 {2,S}

//!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!
//! New work for sec- and tert-butanol paper:
!
//!    "Accurate Reaction Networks for Alternative Fuels: Butanol
Isomers"      !
//!    K.M. Van Geem, M.R. Harper, S.P. Pyl, G.B. Marin, W.H. Green
!
```

```
//!    To be submitted to Industrial & Engineering Chemical Research
!
//!       for the ISCRE-21 conference
!
//!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!!!!!!!!

tBuOH
1 O 0 {2,S}
2 C 0 {1,S} {3,S} {4,S} {5,S}
3 C 0 {2,S}
4 C 0 {2,S}
5 C 0 {2,S}

iC4H8
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 0 {2,S}
4 C 0 {2,S}

HOC[CH2][CH3]2
1 O 0 {2,S}
2 C 0 {1,S} {3,S} {4,S} {5,S}
3 C 1 {2,S}
4 C 0 {2,S}
5 C 0 {2,S}

OC[CH3]3
1 O 1 {2,S}
2 C 0 {1,S} {3,S} {4,S} {5,S}
3 C 0 {2,S}
4 C 0 {2,S}
5 C 0 {2,S}

iC4H7
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 1 {2,S}
4 C 0 {2,S}

HCC[CH3]2
1 C 1 {2,D}
2 C 0 {1,D} {3,S} {4,S}
3 C 0 {2,S}
4 C 0 {2,S}

tC4H9
1 C 1 {2,S} {3,S} {4,S}
2 C 0 {1,S}
3 C 0 {1,S}
4 C 0 {1,S}

iC4H9
1 C 0 {2,S} {3,S} {4,S}
2 C 1 {1,S}
3 C 0 {1,S}
4 C 0 {1,S}
```

```
iC4H10
1 C 0 {2,S} {3,S} {4,S}
2 C 0 {1,S}
3 C 0 {1,S}
4 C 0 {1,S}

sSPC(116)
1  O 0 {2,S} {4,S}
2  O 1 {1,S}
3  C 0 {4,S} {8,S} {9,S} {10,S}
4  C 0 {3,S} {5,S} {11,S} {1,S}
5  C 0 {4,S} {6,S} {7,S} {12,S}
6  C 0 {5,S} {13,S} {14,S} {15,S}
7  O 0 {5,S} {16,S}
8  H 0 {3,S}
9  H 0 {3,S}
10  H 0 {3,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {6,S}
14  H 0 {6,S}
15  H 0 {6,S}
16  H 0 {7,S}

sSPC(46)
1  O 0 {2,S} {5,S}
2  O 1 {1,S}
3  C 0 {4,D} {7,S} {8,S}
4  C 0 {3,D} {5,S} {9,S}
5  C 0 {4,S} {6,S} {10,S} {1,S}
6  C 0 {5,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}


sSPC(56)
1  O 0 {2,S} {3,S}
2  O 1 {1,S}
3  C 0 {4,S} {7,S} {8,S} {1,S}
4  C 0 {3,S} {5,D} {9,S}
5  C 0 {4,D} {6,S} {10,S}
6  C 0 {5,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}
```

```
sSPC(752)
1  O 0 {2,S} {5,S}
2  O 1 {1,S}
3  C 0 {4,S} {7,S} {8,S} {13,S}
4  C 0 {12,D} {3,S} {5,S}
5  C 0 {4,S} {6,S} {14,S} {1,S}
6  C 0 {5,S} {10,S} {11,S} {9,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {6,S}
10  H 0 {6,S}
11  H 0 {6,S}
12  O 0 {4,D}
13  H 0 {3,S}
14  H 0 {5,S}


sSPC(332)
1  O 0 {2,S} {3,S}
2  O 1 {1,S}
3  C 0 {4,S} {7,S} {8,S} {1,S}
4  C 0 {3,S} {5,S} {9,S} {15,S}
5  C 0 {4,S} {6,S} {10,S} {14,S}
6  C 0 {5,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}
14  O 0 {16,S} {5,S}
15  H 0 {4,S}
16  H 0 {14,S}


sSPC(1013)
1  O 0 {2,S} {3,S}
2  O 0 {1,S} {16,S}
3  C 0 {4,S} {7,S} {8,S} {1,S}
4  C 0 {3,S} {5,S} {9,S} {15,S}
5  C 1 {4,S} {6,S} {14,S}
6  C 0 {5,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {14,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}
14  O 0 {5,S} {10,S}
15  H 0 {4,S}
16  H 0 {2,S}


sSPC(1072)
1  O 0 {2,S} {3,S}
```

```
2  O 0 {1,S} {15,S}
3  C 0 {4,S} {7,S} {8,S} {1,S}
4  C 0 {3,S} {5,S} {9,S} {14,S}
5  C 0 {13,D} {4,S} {6,S}
6  C 0 {5,S} {10,S} {11,S} {12,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {6,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  O 0 {5,D}
14  H 0 {4,S}
15  H 0 {2,S}


sSPC(1151)
1  O 1 {2,S}
2  C 0 {3,S} {6,S} {7,S} {1,S}
3  C 0 {2,S} {4,S} {8,S} {13,S}
4  C 0 {12,D} {3,S} {5,S}
5  C 0 {4,S} {9,S} {10,S} {11,S}
6  H 0 {2,S}
7  H 0 {2,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {5,S}
12  O 0 {4,D}
13  H 0 {3,S}


sSPC(1356)
1  O 0 {2,S} {3,S}
2  O 1 {1,S}
3  C 0 {4,S} {6,S} {11,S} {1,S}
4  C 0 {10,D} {3,S} {5,S}
5  C 0 {4,S} {7,S} {8,S} {9,S}
6  H 0 {3,S}
7  H 0 {5,S}
8  H 0 {5,S}
9  H 0 {5,S}
10  O 0 {4,D}
11  H 0 {3,S}


sSPC(1697)
1  O 0 {2,S} {3,S}
2  O 1 {1,S}
3  C 0 {4,S} {5,S} {6,S} {1,S}
4  H 0 {3,S}
5  H 0 {3,S}
6  H 0 {3,S}


sSPC(1735)
1  C 0 {2,S} {3,S} {4,S} {6,S}
```

```
2  H 0 {1,S}
3  H 0 {1,S}
4  H 0 {1,S}
5  O 0 {6,S} {7,S}
6  O 0 {5,S} {1,S}
7  H 0 {5,S}


sSPC(1909)
1  C 1 {2,S} {3,S} {5,S}
2  C 0 {4,D} {1,S} {6,S}
3  H 0 {1,S}
4  O 0 {2,D}
5  H 0 {1,S}
6  O 1 {2,S}


sSPC(3071)
1  O 0 {2,S} {4,S}
2  O 1 {1,S}
3  O 0 {4,D}
4  C 0 {3,D} {5,S} {1,S}
5  H 0 {4,S}


sSPC(3121)
1  O 0 {2,D}
2  C 0 {1,D} {3,S} {5,S}
3  H 0 {2,S}
4  O 0 {5,S} {6,S}
5  O 0 {4,S} {2,S}
6  H 0 {4,S}


sSPC(2810)
1  C 0 {3,D} {2,S} {4,S}
2  O 1 {1,S}
3  O 0 {1,D}
4  H 0 {1,S}



sSPC(1474)
1  C 0 {2,S} {4,S} {9,S} {11,S}
2  C 0 {8,D} {1,S} {3,S}
3  C 0 {2,S} {5,S} {6,S} {7,S}
4  H 0 {1,S}
5  H 0 {3,S}
6  H 0 {3,S}
7  H 0 {3,S}
8  O 0 {2,D}
9  H 0 {1,S}
10  O 0 {11,S} {12,S}
11  O 0 {10,S} {1,S}
12  H 0 {10,S}
```

```
sSPC(1590)
1  O 1 {2,S}
2  C 0 {3,S} {5,S} {10,S} {1,S}
3  C 0 {9,D} {2,S} {4,S}
4  C 0 {3,S} {6,S} {7,S} {8,S}
5  H 0 {2,S}
6  H 0 {4,S}
7  H 0 {4,S}
8  H 0 {4,S}
9  O 0 {3,D}
10  H 0 {2,S}


tSPC(54)
1  O 0 {2,S} {5,S}
2  O 1 {1,S}
3  C 0 {4,D} {7,S} {8,S}
4  C 0 {3,D} {5,S} {6,S}
5  C 0 {4,S} {9,S} {10,S} {1,S}
6  C 0 {4,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}


tSPC(77)
1  O 0 {2,S} {5,S}
2  O 0 {1,S} {11,S}
3  C 0 {4,D} {7,S} {8,S}
4  C 0 {3,D} {5,S} {6,S}
5  C 0 {4,S} {9,S} {10,S} {1,S}
6  C 1 {4,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {2,S}
12  H 0 {6,S}
13  H 0 {6,S}


tSPC(122)
1  O 0 {2,S} {8,S}
2  O 1 {1,S}
3  O 0 {4,S} {7,S}
4  O 0 {3,S} {13,S}
5  C 0 {6,D} {9,S} {10,S}
6  C 0 {5,D} {7,S} {8,S}
7  C 0 {6,S} {11,S} {12,S} {3,S}
8  C 0 {6,S} {14,S} {15,S} {1,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {7,S}
```

```
12  H 0 {7,S}
13  H 0 {4,S}
14  H 0 {8,S}
15  H 0 {8,S}


tSPC(157)
1  O 0 {2,S} {8,S}
2  O 0 {1,S} {11,S}
3  O 0 {4,S} {7,S}
4  O 0 {3,S} {13,S}
5  C 1 {6,S} {9,S} {10,S}
6  C 0 {5,S} {7,D} {8,S}
7  C 0 {6,D} {12,S} {3,S}
8  C 0 {6,S} {14,S} {15,S} {1,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {2,S}
12  H 0 {7,S}
13  H 0 {4,S}
14  H 0 {8,S}
15  H 0 {8,S}


tSPC(213)
1  O 0 {2,S} {7,S}
2  O 0 {1,S} {10,S}
3  O 0 {6,D}
4  C 0 {5,D} {8,S} {9,S}
5  C 0 {4,D} {6,S} {7,S}
6  C 0 {3,D} {5,S} {11,S}
7  C 0 {5,S} {12,S} {13,S} {1,S}
8  H 0 {4,S}
9  H 0 {4,S}
10  H 0 {2,S}
11  H 0 {6,S}
12  H 0 {7,S}
13  H 0 {7,S}


tSPC(97)
1  O 0 {2,S} {5,S}
2  O 1 {1,S}
3  C 0 {4,S} {7,S} {8,S} {15,S}
4  C 0 {3,S} {5,S} {6,S} {14,S}
5  C 0 {4,S} {9,S} {10,S} {1,S}
6  C 0 {4,S} {11,S} {12,S} {13,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}
14  O 0 {16,S} {4,S}
15  H 0 {3,S}
16  H 0 {14,S}
```

```
tSPC(439)
1  O 0 {2,S} {5,S}
2  O 0 {1,S} {7,S}
3  C 1 {4,S} {8,S} {15,S}
4  C 0 {3,S} {5,S} {6,S} {14,S}
5  C 0 {4,S} {9,S} {10,S} {1,S}
6  C 0 {4,S} {11,S} {12,S} {13,S}
7  H 0 {2,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {6,S}
12  H 0 {6,S}
13  H 0 {6,S}
14  O 0 {16,S} {4,S}
15  H 0 {3,S}
16  H 0 {14,S}


tSPC(343)
1  O 1 {6,S}
2  O 0 {5,D}
3  C 0 {4,D} {7,S} {8,S}
4  C 0 {3,D} {5,S} {6,S}
5  C 0 {2,D} {4,S} {9,S}
6  C 0 {4,S} {10,S} {11,S} {1,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {5,S}
10  H 0 {6,S}
11  H 0 {6,S}


tSPC(346)
1  O 0 {4,D}
2  C 0 {3,D} {5,S} {6,S}
3  C 1 {2,D} {4,S}
4  C 0 {3,S} {7,S} {1,D}
5  H 0 {2,S}
6  H 0 {2,S}
7  H 0 {4,S}


tSPC(878)
1  O 0 {2,S} {5,S}
2  O 1 {1,S}
3  O 0 {6,D}
4  C 0 {5,D} {7,S} {8,S}
5  C 0 {4,D} {6,S} {1,S}
6  C 0 {3,D} {5,S} {9,S}
7  H 0 {4,S}
8  H 0 {4,S}
9  H 0 {6,S}
```

```
H2CCCO
1  O 0 {4,D}
2  C 0 {3,D} {5,S} {6,S}
3  C 0 {2,D} {4,D}
4  C 0 {3,D} {1,D}
5  H 0 {2,S}
6  H 0 {2,S}


tSPC(1286)
1  O 0 {2,S} {6,S}
2  O 1 {1,S}
3  O 0 {6,D}
4  C 0 {5,D} {8,S} {9,S}
5  C 0 {4,D} {6,S} {7,S}
6  C 0 {3,D} {5,S} {1,S}
7  H 0 {5,S}
8  H 0 {4,S}
9  H 0 {4,S}


tSPC(1416)
1  O 0 {4,D}
2  C 0 {3,D} {6,S} {7,S}
3  C 0 {2,D} {4,S} {5,S}
4  C 0 {1,D} {3,S} {9,S}
5  H 0 {3,S}
6  H 0 {2,S}
7  H 0 {2,S}
8  O 0 {9,S} {10,S}
9  O 0 {8,S} {4,S}
10  H 0 {8,S}


tSPC(1553)
1  O 1 {5,S}
2  O 0 {5,D}
3  C 0 {4,D} {7,S} {8,S}
4  C 0 {3,D} {5,S} {6,S}
5  C 0 {2,D} {4,S} {1,S}
6  H 0 {4,S}
7  H 0 {3,S}
8  H 0 {3,S}


C8H14
1  C 0 {2,D} {5,S} {6,S}
2  C 0 {1,D} {3,S} {4,S}
3  C 0 {2,S} {7,S} {8,S} {14,S}
4  C 0 {2,S} {9,S} {10,S} {11,S}
5  H 0 {1,S}
6  H 0 {1,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {4,S}
11  H 0 {4,S}
```

```
12  C 0 {13,D} {16,S} {17,S}
13  C 0 {12,D} {14,S} {15,S}
14  C 0 {13,S} {18,S} {19,S} {3,S}
15  C 0 {13,S} {20,S} {21,S} {22,S}
16  H 0 {12,S}
17  H 0 {12,S}
18  H 0 {14,S}
19  H 0 {14,S}
20  H 0 {15,S}
21  H 0 {15,S}
22  H 0 {15,S}


tSPC(3683)
1  O 0 {2,S} {5,S}
2  O 0 {1,S} {9,S}
3  O 1 {4,S}
4  C 0 {6,D} {3,S} {5,S}
5  C 0 {4,S} {7,S} {8,S} {1,S}
6  C 0 {4,D} {10,S} {11,S}
7  H 0 {5,S}
8  H 0 {5,S}
9  H 0 {2,S}
10  H 0 {6,S}
11  H 0 {6,S}


C4H8O2(62)
1  C 0 {2,D} {5,S} {6,S}
2  C 0 {1,D} {3,S} {4,S}
3  C 0 {2,S} {7,S} {8,S} {13,S}
4  C 0 {2,S} {9,S} {10,S} {11,S}
5  H 0 {1,S}
6  H 0 {1,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {4,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  O 0 {13,S} {14,S}
13  O 0 {12,S} {3,S}
14  H 0 {12,S}


C4H7OJ(79)
1  O 1 {4,S}
2  C 0 {3,D} {6,S} {7,S}
3  C 0 {2,D} {4,S} {5,S}
4  C 0 {3,S} {8,S} {9,S} {1,S}
5  C 0 {3,S} {10,S} {11,S} {12,S}
6  H 0 {2,S}
7  H 0 {2,S}
8  H 0 {4,S}
9  H 0 {4,S}
10  H 0 {5,S}
11  H 0 {5,S}
12  H 0 {5,S}
```

```
tSPC(110)
1  O 1 {4,S}
2  C 1 {3,S} {6,S} {7,S}
3  C 0 {2,S} {4,D} {5,S}
4  C 0 {3,D} {8,S} {1,S}
5  C 0 {3,S} {9,S} {10,S} {11,S}
6  H 0 {2,S}
7  H 0 {2,S}
8  H 0 {4,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {5,S}


C4H6O(105)
1  O 0 {4,S} {2,S}
2  C 0 {3,S} {1,S} {6,S} {7,S}
3  C 0 {2,S} {4,D} {5,S}
4  C 0 {3,D} {1,S} {8,S}
5  C 0 {3,S} {9,S} {10,S} {11,S}
6  H 0 {2,S}
7  H 0 {2,S}
8  H 0 {4,S}
9  H 0 {5,S}
10  H 0 {5,S}
11  H 0 {5,S}

C5H10_iso
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,D}
3 C 0 {2,S} {4,S}
4 C 0 {3,S}
5 C 0 {2,D}

C5H9J(5)
1  C 1 {2,D}
2  C 0 {1,D} {3,S} {4,S}
3  C 0 {2,S}
4  C 0 {2,S} {5,S}
5  C 0 {4,S}

C5H9J(7)
1  C 0 {2,D}
2  C 0 {1,D} {3,S} {4,S}
3  C 1 {2,S}
4  C 0 {2,S} {5,S}
5  C 0 {4,S}

C5H9J(8)
1  C 1 {2,S}
2  C 0 {1,S} {3,S} {4,D}
3  C 0 {2,S}
4  C 0 {2,D} {5,S}
5  C 0 {4,S}
```

```
C5H9J(9)
1  C 0 {2,D}
2  C 0 {1,D} {3,S} {4,S}
3  C 0 {2,S}
4  C 0 {2,S} {5,S}
5  C 1 {4,S}

C5H11J(10)
1 C 1 {2,S} {3,S} {4,S}
2 C 0 {1,S}
3 C 0 {1,S}
4 C 0 {1,S} {5,S}
5 C 0 {4,S}

C5H11J(11)
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {4,S}
3 C 0 {2,S}
4 C 0 {2,S} {5,S}
5 C 0 {4,S}

C5H8(95)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 0 {5,D} {1,S} {3,S}
3  C 0 {4,D} {2,S} {9,S}
4  C 0 {3,D} {10,S} {11,S}
5  C 0 {2,D} {12,S} {13,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {5,S}


SPC(482)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 0 {1,S} {3,S} {5,S} {18,S}
3  C 0 {2,S} {4,S} {9,S} {10,S}
4  C 0 {3,S} {11,S} {12,S} {13,S}
5  C 1 {2,S} {14,S} {15,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {3,S}
11  H 0 {4,S}
12  H 0 {4,S}
13  H 0 {4,S}
14  H 0 {5,S}
15  H 0 {5,S}
16  C 0 {17,D} {19,S} {20,S}
17  C 0 {16,D} {18,D}
18  C 0 {17,D} {21,S} {2,S}
19  H 0 {16,S}
```

```
20  H 0 {16,S}
21  H 0 {18,S}


SPC(483)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 1 {1,S} {3,S} {5,S}
3  C 0 {2,S} {4,S} {9,S} {10,S}
4  C 0 {3,S} {11,S} {12,S} {13,S}
5  C 0 {2,S} {14,S} {15,S} {18,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {3,S}
11  H 0 {4,S}
12  H 0 {4,S}
13  H 0 {4,S}
14  H 0 {5,S}
15  H 0 {5,S}
16  C 0 {17,D} {19,S} {20,S}
17  C 0 {16,D} {18,D}
18  C 0 {17,D} {21,S} {5,S}
19  H 0 {16,S}
20  H 0 {16,S}
21  H 0 {18,S}


C5H7J(504)
1  C 0 {2,S} {3,S} {4,S} {9,S}
2  C 1 {1,S} {5,S} {6,S}
3  H 0 {1,S}
4  H 0 {1,S}
5  H 0 {2,S}
6  H 0 {2,S}
7  C 0 {8,D} {10,S} {11,S}
8  C 0 {7,D} {9,D}
9  C 0 {8,D} {12,S} {1,S}
10  H 0 {7,S}
11  H 0 {7,S}
12  H 0 {9,S}


SPC(493)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 0 {1,S} {3,S} {5,S} {16,S}
3  C 0 {4,D} {2,S} {9,S}
4  C 0 {3,D} {10,S} {11,S}
5  C 1 {2,S} {12,S} {13,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {5,S}
```

```
14  C 0 {15,D} {17,S} {18,S}
15  C 0 {14,D} {16,D}
16  C 0 {15,D} {19,S} {2,S}
17  H 0 {14,S}
18  H 0 {14,S}
19  H 0 {16,S}


SPC(494)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 0 {5,D} {1,S} {3,S}
3  C 0 {2,S} {4,S} {9,S} {16,S}
4  C 1 {3,S} {10,S} {11,S}
5  C 0 {2,D} {12,S} {13,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {5,S}
14  C 0 {15,D} {17,S} {18,S}
15  C 0 {14,D} {16,D}
16  C 0 {15,D} {19,S} {3,S}
17  H 0 {14,S}
18  H 0 {14,S}
19  H 0 {16,S}


SPC(495)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 0 {1,S} {3,D} {5,S}
3  C 0 {2,D} {4,S} {9,S}
4  C 0 {3,S} {10,S} {11,S} {16,S}
5  C 1 {2,S} {12,S} {13,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {5,S}
14  C 0 {15,D} {17,S} {18,S}
15  C 0 {14,D} {16,D}
16  C 0 {15,D} {19,S} {4,S}
17  H 0 {14,S}
18  H 0 {14,S}
19  H 0 {16,S}


SPC(496)
1  C 0 {2,S} {6,S} {7,S} {8,S}
2  C 1 {1,S} {3,S} {5,S}
3  C 0 {4,D} {2,S} {9,S}
4  C 0 {3,D} {10,S} {11,S}
```

```
5  C 0 {2,S} {12,S} {13,S} {16,S}
6  H 0 {1,S}
7  H 0 {1,S}
8  H 0 {1,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {5,S}
13  H 0 {5,S}
14  C 0 {15,D} {17,S} {18,S}
15  C 0 {14,D} {16,D}
16  C 0 {15,D} {19,S} {5,S}
17  H 0 {14,S}
18  H 0 {14,S}
19  H 0 {16,S}


SPC(498)
1  C 0 {2,S} {5,S} {6,S} {15,S}
2  C 1 {1,S} {3,S} {4,S}
3  C 0 {2,S} {7,S} {8,S} {9,S}
4  C 0 {2,S} {10,S} {11,S} {12,S}
5  H 0 {1,S}
6  H 0 {1,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {4,S}
13  C 0 {14,D} {16,S} {17,S}
14  C 0 {13,D} {15,D}
15  C 0 {14,D} {18,S} {1,S}
16  H 0 {13,S}
17  H 0 {13,S}
18  H 0 {15,S}


SPC(499)
1  C 1 {2,S} {5,S} {6,S}
2  C 0 {1,S} {3,S} {4,S} {15,S}
3  C 0 {2,S} {7,S} {8,S} {9,S}
4  C 0 {2,S} {10,S} {11,S} {12,S}
5  H 0 {1,S}
6  H 0 {1,S}
7  H 0 {3,S}
8  H 0 {3,S}
9  H 0 {3,S}
10  H 0 {4,S}
11  H 0 {4,S}
12  H 0 {4,S}
13  C 0 {14,D} {16,S} {17,S}
14  C 0 {13,D} {15,D}
15  C 0 {14,D} {18,S} {2,S}
16  H 0 {13,S}
17  H 0 {13,S}
18  H 0 {15,S}
```

```
C6H7J(511)
1  C 0 {3,D} {2,S} {10,S}
2  C 1 {1,S} {4,S} {5,S}
3  C 0 {1,D} {6,S} {7,S}
4  H 0 {2,S}
5  H 0 {2,S}
6  H 0 {3,S}
7  H 0 {3,S}
8  C 0 {9,D} {11,S} {12,S}
9  C 0 {8,D} {10,D}
10  C 0 {9,D} {13,S} {1,S}
11  H 0 {8,S}
12  H 0 {8,S}
13  H 0 {10,S}


C6H7J(512)
1  C 1 {2,S} {3,D}
2  C 0 {1,S} {4,S} {5,S} {10,S}
3  C 0 {1,D} {6,S} {7,S}
4  H 0 {2,S}
5  H 0 {2,S}
6  H 0 {3,S}
7  H 0 {3,S}
8  C 0 {9,D} {11,S} {12,S}
9  C 0 {8,D} {10,D}
10  C 0 {9,D} {13,S} {2,S}
11  H 0 {8,S}
12  H 0 {8,S}
13  H 0 {10,S}


C6H7J(505)
1  C 0 {2,S} {4,S} {5,S} {6,S}
2  C 0 {1,S} {3,D} {10,S}
3  C 1 {2,D} {7,S}
4  H 0 {1,S}
5  H 0 {1,S}
6  H 0 {1,S}
7  H 0 {3,S}
8  C 0 {9,D} {11,S} {12,S}
9  C 0 {8,D} {10,D}
10  C 0 {9,D} {13,S} {2,S}
11  H 0 {8,S}
12  H 0 {8,S}
13  H 0 {10,S}


C6H7J(506)
1  C 0 {2,S} {4,S} {5,S} {6,S}
2  C 1 {1,S} {3,D}
3  C 0 {2,D} {7,S} {10,S}
4  H 0 {1,S}
5  H 0 {1,S}
6  H 0 {1,S}
```

```
7  H 0 {3,S}
8  C 0 {9,D} {11,S} {12,S}
9  C 0 {8,D} {10,D}
10  C 0 {9,D} {13,S} {3,S}
11  H 0 {8,S}
12  H 0 {8,S}
13  H 0 {10,S}


C8H13J(41)
1  C 0 {2,S} {9,S} {10,S} {11,S}
2  C 0 {1,S} {3,D} {5,S}
3  C 0 {2,D} {4,S} {12,S}
4  C 0 {3,S} {6,S} {13,S} {14,S}
5  C 1 {2,S} {15,S} {16,S}
6  C 0 {8,D} {4,S} {7,S}
7  C 0 {6,S} {17,S} {18,S} {19,S}
8  C 0 {6,D} {20,S} {21,S}
9  H 0 {1,S}
10  H 0 {1,S}
11  H 0 {1,S}
12  H 0 {3,S}
13  H 0 {4,S}
14  H 0 {4,S}
15  H 0 {5,S}
16  H 0 {5,S}
17  H 0 {7,S}
18  H 0 {7,S}
19  H 0 {7,S}
20  H 0 {8,S}
21  H 0 {8,S}


C8H15J(44)
1  C 0 {2,S} {9,S} {10,S} {11,S}
2  C 1 {1,S} {3,S} {5,S}
3  C 0 {2,S} {4,S} {12,S} {13,S}
4  C 0 {3,S} {6,S} {14,S} {15,S}
5  C 0 {2,S} {16,S} {17,S} {23,S}
6  C 0 {8,D} {4,S} {7,S}
7  C 0 {6,S} {18,S} {19,S} {20,S}
8  C 0 {6,D} {21,S} {22,S}
9  H 0 {1,S}
10  H 0 {1,S}
11  H 0 {1,S}
12  H 0 {3,S}
13  H 0 {3,S}
14  H 0 {4,S}
15  H 0 {4,S}
16  H 0 {5,S}
17  H 0 {5,S}
18  H 0 {7,S}
19  H 0 {7,S}
20  H 0 {7,S}
21  H 0 {8,S}
22  H 0 {8,S}
23  H 0 {5,S}
```

```
SPC(425)
1  C 0 {2,S} {9,S} {10,S} {11,S}
2  C 0 {1,S} {3,S} {5,S} {25,S}
3  C 0 {2,S} {4,S} {12,S} {13,S}
4  C 0 {3,S} {6,S} {14,S} {15,S}
5  C 1 {2,S} {16,S} {17,S}
6  C 0 {8,D} {4,S} {7,S}
7  C 0 {6,S} {18,S} {19,S} {20,S}
8  C 0 {6,D} {21,S} {22,S}
9  H 0 {1,S}
10  H 0 {1,S}
11  H 0 {1,S}
12  H 0 {3,S}
13  H 0 {3,S}
14  H 0 {4,S}
15  H 0 {4,S}
16  H 0 {5,S}
17  H 0 {5,S}
18  H 0 {7,S}
19  H 0 {7,S}
20  H 0 {7,S}
21  H 0 {8,S}
22  H 0 {8,S}
23  C 0 {24,D} {26,S} {27,S}
24  C 0 {23,D} {25,D}
25  C 0 {24,D} {28,S} {2,S}
26  H 0 {23,S}
27  H 0 {23,S}
28  H 0 {25,S}


SPC(426)
1  C 0 {2,S} {9,S} {10,S} {11,S}
2  C 1 {1,S} {3,S} {5,S}
3  C 0 {2,S} {4,S} {12,S} {13,S}
4  C 0 {3,S} {6,S} {14,S} {15,S}
5  C 0 {2,S} {16,S} {17,S} {25,S}
6  C 0 {8,D} {4,S} {7,S}
7  C 0 {6,S} {18,S} {19,S} {20,S}
8  C 0 {6,D} {21,S} {22,S}
9  H 0 {1,S}
10  H 0 {1,S}
11  H 0 {1,S}
12  H 0 {3,S}
13  H 0 {3,S}
14  H 0 {4,S}
15  H 0 {4,S}
16  H 0 {5,S}
17  H 0 {5,S}
18  H 0 {7,S}
19  H 0 {7,S}
20  H 0 {7,S}
21  H 0 {8,S}
22  H 0 {8,S}
23  C 0 {24,D} {26,S} {27,S}
```

```
24  C 0 {23,D} {25,D}
25  C 0 {24,D} {28,S} {5,S}
26  H 0 {23,S}
27  H 0 {23,S}
28  H 0 {25,S}


C7H10(454)
1  C 0 {2,S} {4,S} {5,S} {9,S}
2  C 0 {1,S} {3,T}
3  C 0 {2,T} {6,S}
4  H 0 {1,S}
5  H 0 {1,S}
6  H 0 {3,S}
7  C 0 {8,S} {11,S} {12,S} {13,S}
8  C 0 {10,D} {7,S} {9,S}
9  C 0 {8,S} {14,S} {15,S} {1,S}
10  C 0 {8,D} {16,S} {17,S}
11  H 0 {7,S}
12  H 0 {7,S}
13  H 0 {7,S}
14  H 0 {9,S}
15  H 0 {9,S}
16  H 0 {10,S}
17  H 0 {10,S}


CH3CHCHCHO
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

CHCHCHO
1 C 1 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

CH3CCHCHO
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

CH3CHCHCO
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 1 {3,S} {5,D}
5 O 0 {4,D}

C4H7O-14
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
```

```
3 C 0 {2,S} {4,S}
4 C 1 {3,S} {5,S}
5 O 0 {4,S}

C12H10
1 C 0 {3,D} {4,S}
2 C 0 {5,D} {6,S}
3 C 0 {1,D} {7,S}
4 C 0 {1,S} {8,D}
5 C 0 {2,D} {9,S}
6 C 0 {2,S} {10,D}
7 C 0 {3,S} {11,D}
8 C 0 {4,D} {11,S}
9 C 0 {5,S} {12,D}
10 C 0 {6,D} {12,S}
11 C 0 {7,D} {8,S} {12,S}
12 C 0 {9,D} {10,S} {11,S}

biC5H5
1 C 0 {2,S} {5,D}
2 C 0 {1,S} {6,D}
3 C 0 {4,S} {7,D}
4 C 0 {3,S} {8,D}
5 C 0 {1,D} {9,S}
6 C 0 {2,D} {9,S}
7 C 0 {3,D} {10,S}
8 C 0 {4,D} {10,S}
9 C 0 {5,S} {6,S} {10,S}
10 C 0 {7,S} {8,S} {9,S}

C5H4C5H5
1 C 0 {2,S} {5,D}
2 C 0 {1,S} {6,D}
3 C 0 {4,D} {7,S}
4 C 0 {3,D} {8,S}
5 C 0 {1,D} {9,S}
6 C 0 {2,D} {9,S}
7 C 0 {3,S} {10,D}
8 C 1 {4,S} {10,S}
9 C 0 {5,S} {6,S} {10,S}
10 C 0 {7,D} {8,S} {9,S}

C10H9
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {6,S}
3 C 0 {4,S} {7,D}
4 C 0 {3,S} {8,D}
5 C 1 {1,S} {9,S}
6 C 0 {2,S} {10,D}
7 C 0 {3,D} {9,S}
8 C 0 {4,D} {10,S}
9 C 0 {5,S} {7,S} {10,S}
10 C 0 {6,D} {8,S} {9,S}

fulvalene
1 C 0 {2,S} {5,D}
2 C 0 {1,S} {6,D}
```

```
3 C 0 {4,S} {7,D}
4 C 0 {3,S} {8,D}
5 C 0 {1,D} {9,S}
6 C 0 {2,D} {9,S}
7 C 0 {3,D} {10,S}
8 C 0 {4,D} {10,S}
9 C 0 {5,S} {6,S} {10,D}
10 C 0 {7,S} {8,S} {9,D}

C10H8
1 C 0 {2,D} {5,S}
2 C 0 {1,D} {6,S}
3 C 0 {4,S} {7,D}
4 C 0 {3,S} {8,D}
5 C 0 {1,S} {9,D}
6 C 0 {2,S} {10,D}
7 C 0 {3,D} {9,S}
8 C 0 {4,D} {10,S}
9 C 0 {5,D} {7,S} {10,S}
10 C 0 {6,D} {8,S} {9,S}

iBuOH
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C3H7O-N2
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

C4H9Oi1
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C4H9Oi2
1 C 0 {2,S}
2 C 1 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C4H9Oi3
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 1 {2,S} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C4H9Oi4
1 C 0 {2,S}
```

```
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 O 1 {3,S}
5 C 0 {2,S}

C4H8O-i1
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C4H8O-i2
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {5,S}
3 C 0 {2,D} {4,S}
4 O 0 {3,S}
5 C 0 {2,S}

C4H8O-i3
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}
5 C 0 {2,S}

iC4H7OJ(15)
1  C 1 {2,S}
2  C 0 {1,S} {3,D} {5,S}
3  C 0 {2,D} {4,S}
4  O 0 {3,S}
5  C 0 {2,S}

iC4H7OJ(17)
1  C 0 {2,D}
2  C 0 {1,D} {3,S} {5,S}
3  C 0 {2,S} {4,S}
4  O 0 {3,S}
5  C 1 {2,S}

iC4H7OJ(30)
1  C 0 {2,S}
2  C 0 {1,S} {3,D} {5,S}
3  C 0 {2,D} {4,S}
4  O 1 {3,S}
5  C 0 {2,S}

iC4H7OJ(48)
1  C 1 {2,S}
2  C 0 {1,S} {3,S} {5,S}
3  C 0 {4,D} {2,S}
4  O 0 {3,D}
5  C 0 {2,S}

iC4H7OJ(51)
1  C 0 {2,S}
2  C 0 {1,S} {3,S} {5,S}
```

```
3  C 1 {2,S} {4,D}
4  O 0 {3,D}
5  C 0 {2,S}

C3H3OH
1 C 0 {2,D}
2 C 0 {1,D} {3,D}
3 C 0 {2,D} {4,S}
4 O 0 {3,S}

C4H6Oi-12
1 C 0 {2,S}
2 C 0 {1,S} {3,D} {5,S}
3 C 0 {2,D} {4,D}
4 O 0 {3,D}
5 C 0 {2,S}

C4H6Oi-13
1 C 0 {2,D}
2 C 0 {1,D} {3,S} {5,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}
5 C 0 {2,S}

iC4H5OJ(14)
1  C 0 {2,D}
2  C 0 {1,D} {3,S} {5,S}
3  C 1 {2,S} {4,D}
4  O 0 {3,D}
5  C 0 {2,S}

iC4H5OJ(15)
1  C 0 {2,D}
2  C 0 {1,D} {3,S} {5,S}
3  C 0 {4,D} {2,S}
4  O 0 {3,D}
5  C 1 {2,S}

C3H3OJ(9)
1  C 1 {2,D}
2  C 0 {1,D} {3,D}
3  C 0 {2,D} {4,S}
4  O 0 {3,S}

HCCCHO
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,D}
4 O 0 {3,D}

C3H3OJ
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,D}
4 O 0 {3,D}

C3H5OJ
```

```
1 C 0 {2,D}
2 C 1 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

C3H5OJ(17)
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 O 0 {3,S}

nC3H7OH
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

C4H7OJ(9)
1 C 1 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

C4H9O2J(52)
1 O 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 C 0 {4,S} {6,S}
6 O 0 {5,S}

C4H9O2J(53)
1 C 1 {2,S}
2 C 0 {1,S} {3,S} {6,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}
6 O 0 {2,S}

C4H9O2J(54)
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {6,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}
6 O 0 {2,S}

C4H9O2J(55)
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S} {6,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}
6 O 0 {3,S}

CH2CHCHCHOH
```

```
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

CHCHCHCHOH
1 C 1 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

CH2CHCCHOH
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

CH2CHCHCOH
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,D}
4 C 1 {3,D} {5,S}
5 O 0 {4,S}

CHCCHCHOH
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

CHCCCHOH
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 1 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}

C4H5O3J(1)
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 0 {4,S} {7,S}
7 O 1 {6,S}

C4H5O3J(2)
1 C 0 {2,S}
2 C 1 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 0 {4,S} {7,S}
```

```
7 O 0 {6,S}

OCOOH
1 O 0 {2,S}
2 O 0 {1,S} {3,S}
3 C 1 {2,S} {4,D}
4 O 0 {3,D}

C4H6O3(21)
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 0 {4,S} {7,S}
7 O 0 {6,S}

C4H5O2J(12)
1 C 0 {2,S}
2 C 0 {1,S} {3,D}
3 C 0 {2,D} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 1 {4,S}

CH2CHCHCHO
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}

C4H6O3(3)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S} {6,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}
6 O 0 {3,S} {7,S}
7 O 0 {6,S}

C4H5O2J(13)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S} {6,S}
4 C 0 {3,S} {5,D}
5 O 0 {4,D}
6 O 1 {3,S}

C4H7O3J(1)
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 0 {4,S} {7,S}
7 O 1 {6,S}
```

```
C4H7O3J(2)
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,D} {6,S}
5 O 0 {4,D}
6 O 0 {4,S} {7,S}
7 O 0 {6,S}

C4H7O3J(3)
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {6,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 0 {4,S}
6 O 0 {2,S} {7,S}
7 O 1 {6,S}

C4H7O3J(4)
1 C 0 {2,S}
2 C 0 {1,S} {3,S} {6,S}
3 C 0 {2,S} {4,D}
4 C 0 {3,D} {5,S}
5 O 1 {4,S}
6 O 0 {2,S} {7,S}
7 O 0 {6,S}

C4H7O3J(5)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S} {6,S}
4 C 0 {3,S} {5,S}
5 O 0 {4,S}
6 O 0 {3,S} {7,S}
7 O 1 {6,S}

C4H7O3J(6)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S} {6,S}
4 C 0 {3,S} {5,S}
5 O 1 {4,S}
6 O 0 {3,S} {7,S}
7 O 0 {6,S}

C3H5O2J(54)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 1 {2,S} {4,S}
4 O 0 {3,S} {5,S}
5 O 0 {4,S}

C4H5O3J(3)
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S} {6,S}
```

```
4 C 0 {3,S} {5,D}
5 O 0 {4,D}
6 O 0 {3,S} {7,S}
7 O 1 {6,S}

CH2CHCH2O
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 1 {3,S}

OCH2CH2CH3
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 O 1 {3,S}

HCOOH
1 C 0 {2,D} {3,S}
2 O 0 {1,D}
3 O 0 {1,S}

CH2OOH
1 C 1 {2,S}
2 O 0 {1,S} {3,S}
3 O 0 {2,S}

HOCHOOH
1 C 1 {2,S} {3,S}
2 O 0 {1,S}
3 O 0 {1,S} {4,S}
4 O 0 {3,S}

C4H5-114
1 C 0 {2,T}
2 C 0 {1,T} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S}

C4H9_2_4
1 C 0 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 C 1 {3,S} {5,S}
5 C 0 {4,S}

CHCHCH2OH
1 C 1 {2,D}
2 C 0 {1,D} {3,S}
3 C 0 {2,S} {4,S}
4 O 0 {3,S}

CCCC(OO)OH
1 C 0 {2,S}
2 C 0 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S} {6,S}
```

```
5 O 0 {4,S}
6 O 0 {4,S} {7,S}
7 O 1 {6,S}

CcCC(OOH)OH
1 C 0 {2,S}
2 C 1 {1,S} {3,S}
3 C 0 {2,S} {4,S}
4 C 0 {3,S} {5,S} {6,S}
5 O 0 {4,S}
6 O 0 {4,S} {7,S}
7 O 0 {6,S}

HOOCH2CO
1 O 0 {2,S}
2 O 0 {1,S} {3,S}
3 C 0 [2,S} {4,S}
4 C 1 {3,S} {5,D}
5 O 0 {4,D}
```

4. Glossary:

H2	InChI=1/H2/h1H
CO2	InChI=1/CO2/c2-1-3
CO	InChI=1/CO/c1-2
CH4	InChI=1/CH4/h1H4
C2H4	InChI=1/C2H4/c1-2/h1-2H2
C2H2	InChI=1/C2H2/c1-2/h1-2H
C2H6	InChI=1/C2H6/c1-2/h1-2H3
C3H6	InChI=1/C3H6/c1-3-2/h3H,1H2,2H3
C3H8	InChI=1/C3H8/c1-3-2/h3H2,1-2H3
aC3H4	InChI=1/C3H4/c1-3-2/h1-2H2
pC3H4	InChI=1/C3H4/c1-3-2/h1H,2H3
CH3OH	InChI=1/CH4O/c1-2/h2H,1H3
C4H8-1	InChI=1/C4H8/c1-3-4-2/h3H,1,4H2,2H3
C4H6-13	InChI=1/C4H6/c1-3-4-2/h3-4H,1-2H2
nC4H10	InChI=1/C4H10/c1-3-4-2/h3-4H2,1-2H3
C2H5OH	InChI=1/C2H6O/c1-2-3/h3H,2H2,1H3
benzene	InChI=1/C6H6/c1-2-4-6-5-3-1/h1-6H
nC4H10O	InChI=1/C4H10O/c1-2-3-4-5/h5H,2-4H2,1H3
C2H3	InChI=1/C2H3/c1-2/h1H,2H2
CH2CO	InChI=1/C2H2O/c1-2-3/h1H2
C2H4O	InChI=1/C2H4O/c1-2-3/h2-3H,1H2
CH3CHO	InChI=1/C2H4O/c1-2-3/h2H,1H3
H2O	InChI=1/H2O/h1H2
nC4H8O	InChI=1/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3
C4H7OJ(8)	InChI=1/C4H7O/c1-2-3-4-5/h2-3H2,1H3
C4H7OJ(12)	InChI=1/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3
C4H7OJ(13)	InChI=1/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3
C4H7OJ(16)	InChI=1/C4H7O/c1-2-3-4-5/h4H,1-3H2
CH2CHO	InChI=1/C2H3O/c1-2-3/h2H,1H2
C3H6O-enol2	InChI=1/C3H6O/c1-2-3-4/h2,4H,1,3H2
C3H5O-enol2	InChI=1/C3H5O/c1-2-3-4/h2-4H,1H2
CH2O	InChI=1/CH2O/c1-2/h1H2
C4H8O-enol	InChI=1/C4H8O/c1-2-3-4-5/h3-5H,2H2,1H3
C4H8O-enol2	InChI=1/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3
C4H8O-enol3	InChI=1/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2
C4H9O-1	InChI=1/C4H9O/c1-2-3-4-5/h5H,1-4H2
C4H9O-2	InChI=1/C4H9O/c1-2-3-4-5/h2,5H,3-4H2,1H3
C4H9O-3	InChI=1/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3
C4H9O-4	InChI=1/C4H9O/c1-2-3-4-5/h4-5H,2-3H2,1H3
C4H9O-5	InChI=1/C4H9O/c1-2-3-4-5/h2-4H2,1H3
C3H7O-N1	InChI=1/C3H7O/c1-2-3-4/h4H,1-3H2
C3H5OJ(8)	InChI=1/C3H5O/c1-2-3-4/h2H2,1H3
C3H5OJ(12)	InChI=1/C3H5O/c1-2-3-4/h2-3H,1H3
C3H5OJ(13)	InChI=1/C3H5O/c1-2-3-4/h3H,1-2H2
C3H6O	InChI=1/C3H6O/c1-2-3-4/h3H,2H2,1H3
C2H5	InChI=1/C2H5/c1-2/h1H2,2H3
H	InChI=1/H
O	InChI=1/O
O2	InChI=1/O2/c1-2
OH	InChI=1/HO/h1H
HO2	InChI=1/HO2/c1-2/h1H
H2O2	InChI=1/H2O2/c1-2/h1-2H
C	InChI=1/C
CH	InChI=1/CH/h1H
CH2	InChI=1/CH2/h1H2

CH2(S)	InChI=1/CH2/h1H2
CH3	InChI=1/CH3/h1H3
HCO	InChI=1/CHO/c1-2/h1H
CH2OH	InChI=1/CH3O/c1-2/h2H,1H2
CH3O	InChI=1/CH3O/c1-2/h1H3
C2H	InChI=1/C2H/c1-2/h1H
HCCO	InChI=1/C2HO/c1-2-3/h1H
HCCOH	InChI=1/C2H2O/c1-2-3/h1,3H
C2O	InChI=1/C2O/c1-2-3
HOC2H4O2	InChI=1/C2H5O3/c3-1-2-5-4/h3H,1-2H2
C3H2	InChI=1/C3H2/c1-3-2/h1-2H
pC3H3	InChI=1/C3H3/c1-3-2/h1H,2H2
aC3H5	InChI=1/C3H5/c1-3-2/h3H,1-2H2
pC3H5	InChI=1/C3H5/c1-3-2/h1,3H,2H3
sC3H5	InChI=1/C3H5/c1-3-2/h1H2,2H3
C3H7-1	InChI=1/C3H7/c1-3-2/h1,3H2,2H3
C3H7-2	InChI=1/C3H7/c1-3-2/h3H,1-2H3
C2H5O-1	InChI=1/C2H5O/c1-2-3/h3H,1-2H2
C2H5O-2	InChI=1/C2H5O/c1-2-3/h2-3H,1H3
C2H5O-3	InChI=1/C2H5O/c1-2-3/h2H2,1H3
C3H4O-enone	InChI=1/C3H4O/c1-2-3-4/h2H,1H3
C3H4O	InChI=1/C3H4O/c1-2-3-4/h2-3H,1H2
C4H7O-13	InChI=1/C4H7O/c1-2-3-4-5/h2-3,5H,1,4H2
C4H2	InChI=1/C4H2/c1-3-4-2/h1-2H
iC4H3	InChI=1/C4H3/c1-3-4-2/h1H,2H2
nC4H3	InChI=1/C4H3/c1-3-4-2/h1-3H
C4H4	InChI=1/C4H4/c1-3-4-2/h1,4H,2H2
C4H5-113	InChI=1/C4H5/c1-3-4-2/h1,4H,2H3
nC4H5	InChI=1/C4H5/c1-3-4-2/h1,3-4H,2H2
iC4H5	InChI=1/C4H5/c1-3-4-2/h3H,1-2H2
C4H6-1	InChI=1/C4H6/c1-3-4-2/h1H,4H2,2H3
C4H6-12	InChI=1/C4H6/c1-3-4-2/h4H,1H2,2H3
C4H7-14	InChI=1/C4H7/c1-3-4-2/h3H,1-2,4H2
C4H7-11	InChI=1/C4H7/c1-3-4-2/h1,3H,4H2,2H3
C4H7-12	InChI=1/C4H7/c1-3-4-2/h1,4H2,2H3
C4H7-24	InChI=1/C4H7/c1-3-4-2/h3-4H,1H2,2H3
C4H9-1	InChI=1/C4H9/c1-3-4-2/h1,3-4H2,2H3
C4H9-2	InChI=1/C4H9/c1-3-4-2/h3H,4H2,1-2H3
C2H3O-1	InChI=1/C2H3O/c1-2-3/h1-3H
C2H3O-2	InChI=1/C2H3O/c1-2-3/h3H,1H2
C6H4	InChI=1/C6H4/c1-2-4-6-5-3-1/h1-4H
C6H5	InChI=1/C6H5/c1-2-4-6-5-3-1/h1-5H
C4H6-2	InChI=1/C4H6/c1-3-4-2/h1-2H3
C4H7-22	InChI=1/C4H7/c1-3-4-2/h3H,1-2H3
CH3CO	InChI=1/C2H3O/c1-2-3/h1H3
C6H10	InChI=1/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2
C6H9_1_2_5	InChI=1/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2
C6H9_CYC_1_3	InChI=1/C6H9/c1-2-4-6-5-3-1/h1-2,5H,3-4,6H2
C6H8_CYC_1_4	InChI=1/C6H8/c1-2-4-6-5-3-1/h1-2,5-6H,3-4H2
C6H7_CYC_1_2	InChI=1/C6H7/c1-2-4-6-5-3-1/h1-5H,6H2
C6H10_CYC	InChI=1/C6H10/c1-2-4-6-5-3-1/h1-2H,3-6H2
C7H9	InChI=1/C7H9/c1-7-5-3-2-4-6-7/h2-5H,6H2,1H3
C8H8	InChI=1/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2
C8H9	InChI=1/C8H9/c1-2-8-6-4-3-5-7-8/h3-7H,1-2H2
C7H8	InChI=1/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3
C3H7O2	InChI=1/C3H7O2/c1-2-3-5-4/h2-3H2,1H3
CH2CH2CH2OOH	InChI=1/C3H7O2/c1-2-3-5-4/h4H,1-3H2

aC3H5O2	InChI=1/C3H5O2/c1-2-3-5-4/h2H,1,3H2
nSPC(301)	InChI=1/C4H9O3/c1-4(7-6)2-3-5/h4-5H,2-3H2,1H3
nSPC(351)	InChI=1/C4H9O3/c1-4(7-6)2-3-5/h3-6H,2H2,1H3
nSPC(385)	InChI=1/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3
nSPC(447)	InChI=1/C4H7O2/c1-4(6)2-3-5/h3-4H,2H2,1H3
nSPC(543)	InChI=1/C2H3O3/c3-1-2-5-4/h1H,2H2
nSPC(801)	InChI=1/C2H3O3/c1-2(3)5-4/h4H,1H2
nSPC(879)	InChI=1/C2H3O5/c3-2(7-5)1-6-4/h5H,1H2
nSPC(1064)	InChI=1/C2H2O4/c3-2(4)1-6-5/h1H2
nSPC(102)	InChI=1/CH2O2/c1-3-2/h1H2
C4H8-2	InChI=1/C4H8/c1-3-4-2/h3-4H,1-2H3
C3H3O-enone	InChI=1/C3H3O/c1-2-3-4/h2H,1H2
FULVENE	InChI=1/C6H6/c1-6-4-2-3-5-6/h2-5H,1H2
C6H5O	InChI=1/C6H5O/c7-6-4-2-1-3-5-6/h1-5H
C5H5	InChI=1/C5H5/c1-2-4-5-3-1/h1-5H
C6H5OH	InChI=1/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H
cyC5H6	InChI=1/C5H6/c1-2-4-5-3-1/h1-4H,5H2
C5H5CH3_1	InChI=1/C6H8/c1-6-4-2-3-5-6/h2-6H,1H3
C5H5CH3_2	InChI=1/C6H8/c1-6-4-2-3-5-6/h2-4H,5H2,1H3
C5H5CH3_3	InChI=1/C6H8/c1-6-4-2-3-5-6/h2,4-5H,3H2,1H3
C8H6	InChI=1/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H
C6H5CH2	InChI=1/C7H7/c1-7-5-3-2-4-6-7/h2-6H,1H2
C6H5CCH2	InChI=1/C8H7/c1-2-8-6-4-3-5-7-8/h3-7H,1H2
C5H4CH3	InChI=1/C6H7/c1-6-4-2-3-5-6/h2-5H,1H3
C5H5CH2-1	InChI=1/C6H7/c1-6-4-2-3-5-6/h2-6H,1H2
C5H5CH2-2	InChI=1/C6H7/c1-6-4-2-3-5-6/h2-4H,1,5H2
C5H5CH2-3	InChI=1/C6H7/c1-6-4-2-3-5-6/h2,4-5H,1,3H2
ME2CYBE	InChI=1/C6H6/c1-5-3-4-6(5)2/h3-4H,1-2H2
c5h4chchch2	InChI=1/C8H8/c1-2-5-8-6-3-4-7-8/h2-7H,1H2
C#CCCC#C	InChI=1/C6H6/c1-3-5-6-4-2/h1-2H,5-6H2
C*C*CC*C*C	InChI=1/C6H6/c1-3-5-6-4-2/h5-6H,1-2H2
CH3CCCH2	InChI=1/C4H5/c1-3-4-2/h1H2,2H3
C4H4-123	InChI=1/C4H4/c1-3-4-2/h1-2H2
C5H10_1	InChI=1/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3
C5H9_1_4	InChI=1/C5H9/c1-3-5-4-2/h3H,1-2,4-5H2
C5H8_CYC_1	InChI=1/C5H8/c1-2-4-5-3-1/h1-2H,3-5H2
C5H9_CYC	InChI=1/C5H9/c1-2-4-5-3-1/h1H,2-5H2
C5H7_CYC_1_2	InChI=1/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2
C4H7O_1_2	InChI=1/C4H7O/c1-2-3-4-5/h2-5H,1H3
sBuOH	InChI=1/C4H10O/c1-3-4(2)5/h4-5H,3H2,1-2H3
CH3C[OH]C2H5	InChI=1/C4H9O/c1-3-4(2)5/h5H,3H2,1-2H3
CH3CH[OH]CHCH3	InChI=1/C4H9O/c1-3-4(2)5/h3-5H,1-2H3
CH3CH[O]C2H5	InChI=1/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3
CH2CH[OH]C2H5	InChI=1/C4H9O/c1-3-4(2)5/h4-5H,2-3H2,1H3
CH3CH[OH]CH2CH2	InChI=1/C4H9O/c1-3-4(2)5/h4-5H,1,3H2,2H3
CH3CH[OH]CH2	InChI=1/C3H7O/c1-3(2)4/h3-4H,1H2,2H3
HOCHC2H5	InChI=1/C3H7O/c1-2-3-4/h3-4H,2H2,1H3
H2CCCH3[OH]	InChI=1/C3H6O/c1-3(2)4/h4H,1H2,2H3
CH3CH-O-CH3	InChI=1/C3H7O/c1-3-4-2/h3H,1-2H3
CH3C[OH]CH3	InChI=1/C3H7O/c1-3(2)4/h4H,1-2H3
acetone	InChI=1/C3H6O/c1-3(2)4/h1-2H3
C2H5CHCHCH2	InChI=1/C5H9/c1-3-5-4-2/h3,5H,1,4H2,2H3
CH2C[OH]CH2	InChI=1/C3H5O/c1-3(2)4/h4H,1-2H2
CH2C[O]CH3	InChI=1/C3H5O/c1-3(2)4/h1H2,2H3
CH3-O-C(CH3)2	InChI=1/C4H9O/c1-4(2)5-3/h1-3H3
C3H6O-enol	InChI=1/C3H6O/c1-2-3-4/h2-4H,1H3
MEK	InChI=1/C4H8O/c1-3-4(2)5/h3H2,1-2H3

sC4H8O	InChI=1/C4H8O/c1-3-4(2)5/h3-5H,1H2,2H3
C4H6O(717)	InChI=1/C4H6O/c1-3-4(2)5/h3H,1H2,2H3
cH2C[O]C2H5	InChI=1/C4H7O/c1-3-4(2)5/h2-3H2,1H3
CH3C[O]cHCH3	InChI=1/C4H7O/c1-3-4(2)5/h3H,1-2H3
CH3C[O]CH2cH2	InChI=1/C4H7O/c1-3-4(2)5/h1,3H2,2H3
MEKenol2	InChI=1/C4H8O/c1-3-4(2)5/h5H,2-3H2,1H3
CH2C[OH]cHCH3	InChI=1/C4H7O/c1-3-4(2)5/h3,5H,2H2,1H3
CH2C[OH]CH2cH2	InChI=1/C4H7O/c1-3-4(2)5/h5H,1-3H2
cHC[OH]C2H5	InChI=1/C4H7O/c1-3-4(2)5/h2,5H,3H2,1H3
MEKenol	InChI=1/C4H8O/c1-3-4(2)5/h3,5H,1-2H3
CH3CHcOH	InChI=1/C3H5O/c1-2-3-4/h2,4H,1H3
CH3C[OH]cH	InChI=1/C3H5O/c1-3(2)4/h1,4H,2H3
CH3C[OH]cCH3	InChI=1/C4H7O/c1-3-4(2)5/h5H,1-2H3
CH3C[OH]CHcH2	InChI=1/C4H7O/c1-3-4(2)5/h3,5H,1H2,2H3
cH2CH[OH]C2H3	InChI=1/C4H7O/c1-3-4(2)5/h3-5H,1-2H2
CH3CH[OH]cCH2	InChI=1/C4H7O/c1-3-4(2)5/h4-5H,1H2,2H3
CH3CH[OH]CHcH	InChI=1/C4H7O/c1-3-4(2)5/h1,3-5H,2H3
CH3CH[o]C2H3	InChI=1/C4H7O/c1-3-4(2)5/h3-4H,1H2,2H3
tBuOH	InChI=1/C4H10O/c1-4(2,3)5/h5H,1-3H3
iC4H8	InChI=1/C4H8/c1-4(2)3/h1H2,2-3H3
HOC[CH2][CH3]2	InChI=1/C4H9O/c1-4(2,3)5/h5H,1H2,2-3H3
OC[CH3]3	InChI=1/C4H9O/c1-4(2,3)5/h1-3H3
iC4H7	InChI=1/C4H7/c1-4(2)3/h1-2H2,3H3
HCC[CH3]2	InChI=1/C4H7/c1-4(2)3/h1H,2-3H3
tC4H9	InChI=1/C4H9/c1-4(2)3/h1-3H3
iC4H9	InChI=1/C4H9/c1-4(2)3/h4H,1H2,2-3H3
iC4H10	InChI=1/C4H10/c1-4(2)3/h4H,1-3H3
sSPC(116)	InChI=1/C4H9O3/c1-3(5)4(2)7-6/h3-5H,1-2H3
sSPC(46)	InChI=1/C4H7O2/c1-3-4(2)6-5/h3-4H,1H2,2H3
sSPC(56)	InChI=1/C4H7O2/c1-2-3-4-6-5/h2-3H,4H2,1H3
sSPC(752)	InChI=1/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3
sSPC(332)	InChI=1/C4H9O3/c1-4(5)2-3-7-6/h4-5H,2-3H2,1H3
sSPC(1013)	InChI=1/C4H9O3/c1-4(5)2-3-7-6/h5-6H,2-3H2,1H3
sSPC(1072)	InChI=1/C4H8O3/c1-4(5)2-3-7-6/h6H,2-3H2,1H3
sSPC(1151)	InChI=1/C4H7O2/c1-4(6)2-3-5/h2-3H2,1H3
sSPC(1356)	InChI=1/C3H5O3/c1-3(4)2-6-5/h2H2,1H3
sSPC(1697)	InChI=1/CH3O2/c1-3-2/h1H3
sSPC(1735)	InChI=1/CH4O2/c1-3-2/h2H,1H3
sSPC(1909)	InChI=1/C2H2O2/c1-2(3)4/h1H2
sSPC(3071)	InChI=1/CHO3/c2-1-4-3/h1H
sSPC(3121)	InChI=1/CH2O3/c2-1-4-3/h1,3H
sSPC(2810)	InChI=1/CHO2/c2-1-3/h1H
sSPC(1474)	InChI=1/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3
sSPC(1590)	InChI=1/C3H5O2/c1-3(5)2-4/h2H2,1H3
tSPC(54)	InChI=1/C4H7O2/c1-4(2)3-6-5/h1,3H2,2H3
tSPC(77)	InChI=1/C4H7O2/c1-4(2)3-6-5/h5H,1-3H2
tSPC(122)	InChI=1/C4H7O4/c1-4(2-7-5)3-8-6/h5H,1-3H2
tSPC(157)	InChI=1/C4H7O4/c1-4(2-7-5)3-8-6/h2,5-6H,1,3H2
tSPC(213)	InChI=1/C4H6O3/c1-4(2-5)3-7-6/h2,6H,1,3H2
tSPC(97)	InChI=1/C4H9O3/c1-4(2,5)3-7-6/h5H,3H2,1-2H3
tSPC(439)	InChI=1/C4H9O3/c1-4(2,5)3-7-6/h5-6H,1,3H2,2H3
tSPC(343)	InChI=1/C4H5O2/c1-4(2-5)3-6/h2H,1,3H2
tSPC(346)	InChI=1/C3H3O/c1-2-3-4/h3H,1H2
tSPC(878)	InChI=1/C3H3O3/c1-3(2-4)6-5/h2H,1H2
H2CCCO	InChI=1/C3H2O/c1-2-3-4/h1H2
tSPC(1286)	InChI=1/C3H3O3/c1-2-3(4)6-5/h2H,1H2
tSPC(1416)	InChI=1/C3H4O3/c1-2-3(4)6-5/h2,5H,1H2

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tSPC(1553)        InChI=1/C3H3O2/c1-2-3(4)5/h2H,1H2
C8H14             InChI=1/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3
tSPC(3683)        InChI=1/C3H5O3/c1-3(4)2-6-5/h5H,1-2H2
C4H8O2(62)        InChI=1/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3
C4H7OJ(79)        InChI=1/C4H7O/c1-4(2)3-5/h1,3H2,2H3
tSPC(110)         InChI=1/C4H6O/c1-4(2)3-5/h3H,1H2,2H3
C4H6O(105)        InChI=1/C4H6O/c1-4-2-5-3-4/h2H,3H2,1H3
C5H10_iso         InChI=1/C5H10/c1-4-5(2)3/h2,4H2,1,3H3
C5H9J(5)          InChI=1/C5H9/c1-4-5(2)3/h2H,4H2,1,3H3
C5H9J(7)          InChI=1/C5H9/c1-4-5(2)3/h2-4H2,1H3
C5H9J(8)          InChI=1/C5H9/c1-4-5(2)3/h4H,2H2,1,3H3
C5H9J(9)          InChI=1/C5H9/c1-4-5(2)3/h1-2,4H2,3H3
C5H11J(10)        InChI=1/C5H11/c1-4-5(2)3/h4H2,1-3H3
C5H11J(11)        InChI=1/C5H11/c1-4-5(2)3/h5H,2,4H2,1,3H3
C5H8(95)          InChI=1/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3
SPC(482)          InChI=1/C8H13/c1-5-7-8(3,4)6-2/h7H,1,3,6H2,2,4H3
SPC(483)          InChI=1/C8H13/c1-4-6-7-8(3)5-2/h6H,1,5,7H2,2-3H3
C5H7J(504)        InChI=1/C5H7/c1-3-5-4-2/h5H,1-3H2
SPC(493)          InChI=1/C8H11/c1-5-7-8(3,4)6-2/h6-7H,1-3H2,4H3
SPC(494)          InChI=1/C8H11/c1-5-6-8(4)7(2)3/h6,8H,1-2,4H2,3H3
SPC(495)          InChI=1/C8H11/c1-4-5-6-7-8(2)3/h5,7H,1-2,6H2,3H3
SPC(496)          InChI=1/C8H11/c1-4-6-7-8(3)5-2/h5-6H,1-2,7H2,3H3
SPC(498)          InChI=1/C7H11/c1-4-5-6-7(2)3/h5H,1,6H2,2-3H3
SPC(499)          InChI=1/C7H11/c1-5-6-7(2,3)4/h6H,1-2H2,3-4H3
C6H7J(511)        InChI=1/C6H7/c1-4-5-6(2)3/h5H,1-3H2
C6H7J(512)        InChI=1/C6H7/c1-3-5-6-4-2/h5H,1-2,6H2
C6H7J(505)        InChI=1/C6H7/c1-4-5-6(2)3/h2,5H,1H2,3H3
C6H7J(506)        InChI=1/C6H7/c1-3-5-6-4-2/h5-6H,1H2,2H3
C8H13J(41)        InChI=1/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3
C8H15J(44)        InChI=1/C8H15/c1-7(2)5-6-8(3)4/h1,5-6H2,2-4H3
SPC(425)          InChI=1/C11H17/c1-6-8-11(4,5)9-7-10(2)3/h8H,1-
2,4,7,9H2,3,5H3
SPC(426)          InChI=1/C11H17/c1-5-6-7-11(4)9-8-10(2)3/h6H,1-2,7-
9H2,3-4H3
C7H10(454)        InChI=1/C7H10/c1-4-5-6-7(2)3/h1H,2,5-6H2,3H3
CH3CHCHCHO        InChI=1/C4H6O/c1-2-3-4-5/h2-4H,1H3
CHCHCHO           InChI=1/C3H3O/c1-2-3-4/h1-3H
CH3CCHCHO         InChI=1/C4H5O/c1-2-3-4-5/h3-4H,1H3
CH3CHCHCO         InChI=1/C4H5O/c1-2-3-4-5/h2-3H,1H3
C4H7O-14          InChI=1/C4H7O/c1-2-3-4-5/h2,4-5H,1,3H2
C12H10            InChI=1/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H
biC5H5            InChI=1/C10H10/c1-2-6-9(5-1)10-7-3-4-8-10/h1-10H
C5H4C5H5          InChI=1/C10H9/c1-2-6-9(5-1)10-7-3-4-8-10/h1-9H
C10H9             InChI=1/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-9H
fulvalene         InChI=1/C10H8/c1-2-6-9(5-1)10-7-3-4-8-10/h1-8H
C10H8             InChI=1/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H
iBuOH             InChI=1/C4H10O/c1-4(2)3-5/h4-5H,3H2,1-2H3
C3H7O-N2          InChI=1/C3H7O/c1-2-3-4/h2,4H,3H2,1H3
C4H9Oi1           InChI=1/C4H9O/c1-4(2)3-5/h4-5H,1,3H2,2H3
C4H9Oi2           InChI=1/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3
C4H9Oi3           InChI=1/C4H9O/c1-4(2)3-5/h3-5H,1-2H3
C4H9Oi4           InChI=1/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3
C4H8O-i1          InChI=1/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3
C4H8O-i2          InChI=1/C4H8O/c1-4(2)3-5/h3,5H,1-2H3
C4H8O-i3          InChI=1/C4H8O/c1-4(2)3-5/h3-4H,1-2H3
iC4H7OJ(15)       InChI=1/C4H7O/c1-4(2)3-5/h3,5H,1H2,2H3
iC4H7OJ(17)       InChI=1/C4H7O/c1-4(2)3-5/h5H,1-3H2
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iC4H7OJ(30)	InChI=1/C4H7O/c1-4(2)3-5/h3H,1-2H3
iC4H7OJ(48)	InChI=1/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3
iC4H7OJ(51)	InChI=1/C4H7O/c1-4(2)3-5/h4H,1-2H3
C3H3OH	InChI=1/C3H4O/c1-2-3-4/h3-4H,1H2
C4H6Oi-12	InChI=1/C4H6O/c1-4(2)3-5/h1-2H3
C4H6Oi-13	InChI=1/C4H6O/c1-4(2)3-5/h3H,1H2,2H3
iC4H5OJ(14)	InChI=1/C4H5O/c1-4(2)3-5/h1H2,2H3
iC4H5OJ(15)	InChI=1/C4H5O/c1-4(2)3-5/h3H,1-2H2
C3H3OJ(9)	InChI=1/C3H3O/c1-2-3-4/h1,3-4H
HCCCHO	InChI=1/C3H2O/c1-2-3-4/h1,3H
C3H3OJ	InChI=1/C3H3O/c1-2-3-4/h1H3
C3H5OJ	InChI=1/C3H5O/c1-2-3-4/h4H,1,3H2
C3H5OJ(17)	InChI=1/C3H5O/c1-2-3-4/h3-4H,1H3
nC3H7OH	InChI=1/C3H8O/c1-2-3-4/h4H,2-3H2,1H3
C4H7OJ(9)	InChI=1/C4H7O/c1-2-3-4-5/h3-5H,1-2H2
C4H9O2J(52)	InChI=1/C4H9O2/c5-3-1-2-4-6/h1,5-6H,2-4H2
C4H9O2J(53)	InChI=1/C4H9O2/c1-4(6)2-3-5/h4-6H,1-3H2
C4H9O2J(54)	InChI=1/C4H9O2/c1-4(6)2-3-5/h2,4-6H,3H2,1H3
C4H9O2J(55)	InChI=1/C4H9O2/c1-2-4(6)3-5/h2,4-6H,3H2,1H3
CH2CHCHCHOH	InChI=1/C4H6O/c1-2-3-4-5/h2-5H,1H2
CHCHCHCHOH	InChI=1/C4H5O/c1-2-3-4-5/h1-5H
CH2CHCCHOH	InChI=1/C4H5O/c1-2-3-4-5/h2,4-5H,1H2
CH2CHCHCOH	InChI=1/C4H5O/c1-2-3-4-5/h2-3,5H,1H2
CHCCHCHOH	InChI=1/C4H4O/c1-2-3-4-5/h1,3-5H
CHCCCHOH	InChI=1/C4H3O/c1-2-3-4-5/h1,4-5H
C4H5O3J(1)	InChI=1/C4H5O3/c1-2-3-4(5)7-6/h2-3H,1H3
C4H5O3J(2)	InChI=1/C4H5O3/c1-2-3-4(5)7-6/h3,6H,1H3
OCOOH	InChI=1/CHO3/c2-1-4-3/h3H
C4H6O3(21)	InChI=1/C4H6O3/c1-2-3-4(5)7-6/h2-3,6H,1H3
C4H5O2J(12)	InChI=1/C4H5O2/c1-2-3-4(5)6/h2-3H,1H3
CH2CHCHCHO	InChI=1/C4H5O/c1-2-3-4-5/h2-4H,1H2
C4H6O3(3)	InChI=1/C4H6O3/c1-2-4(3-5)7-6/h2-4,6H,1H2
C4H5O2J(13)	InChI=1/C4H5O2/c1-2-4(6)3-5/h2-4H,1H2
C4H7O3J(1)	InChI=1/C4H7O3/c1-2-3-4(5)7-6/h2-3H2,1H3
C4H7O3J(2)	InChI=1/C4H7O3/c1-2-3-4(5)7-6/h2,6H,3H2,1H3
C4H7O3J(3)	InChI=1/C4H7O3/c1-4(7-6)2-3-5/h2-5H,1H3
C4H7O3J(4)	InChI=1/C4H7O3/c1-4(7-6)2-3-5/h2-4,6H,1H3
C4H7O3J(5)	InChI=1/C4H7O3/c1-2-4(3-5)7-6/h2,4-5H,1,3H2
C4H7O3J(6)	InChI=1/C4H7O3/c1-2-4(3-5)7-6/h2,4,6H,1,3H2
C3H5O2J(54)	InChI=1/C3H5O2/c1-2-3-5-4/h2-4H,1H2
C4H5O3J(3)	InChI=1/C4H5O3/c1-2-4(3-5)7-6/h2-4H,1H2
CH2CHCH2O	InChI=1/C3H5O/c1-2-3-4/h2H,1,3H2
OCH2CH2CH3	InChI=1/C3H7O/c1-2-3-4/h2-3H2,1H3
HCOOH	InChI=1/CH2O2/c2-1-3/h1H,(H,2,3)/f/h2H
CH2OOH	InChI=1/CH3O2/c1-3-2/h2H,1H2
HOCHOOH	InChI=1/CH3O3/c2-1-4-3/h1-3H
C4H5-114	InChI=1/C4H5/c1-3-4-2/h1H,2,4H2
C4H9_2_4	InChI=1/C5H9/c1-3-5-4-2/h3-4H,1,5H2,2H3
CHCHCH2OH	InChI=1/C3H5O/c1-2-3-4/h1-2,4H,3H2
CCCC(OO)OH	InChI=1/C4H9O3/c1-2-3-4(5)7-6/h4-5H,2-3H2,1H3
CcCC(OOH)OH	InChI=1/C4H9O3/c1-2-3-4(5)7-6/h2,4-6H,3H2,1H3
HOOCH2CO	InChI=1/C2H3O3/c3-1-2-5-4/h4H,2H2

5. Temperature Profiles:

The experimentally measured temperature profiles for the three flames reported in this study as a function of distance from the burner (see text in Section 3).

Distance from Burner / mm	Temperature / K		
	Flame 1	Flame 2	Flame 3
0	500	500	500
0.5	725	504	715
1	955	549	923
1.5	1110	630	1123
2	1232	760	1295
2.5	1345	929	1439
3	1449	1103	1603
3.5	1504	1287	1730
4	1568	1484	1836
4.5	1624	1652	1925
5	1679	1770	2016
5.5	1716	1846	2108
6	1765	1898	2180
6.5	1805	1945	2211
7	1836	1966	2238
7.5	1871	1979	2238
8	1893	1985	2235
9	1933	1984	2224
10	1952	1977	2204
11	1954	1969	2192
12	1946	1958	2181
14	1930	1943	2158
16	1899	1921	2139
18	1874	1898	2117
20	1845	1871	2099
22	1826	1857	2081
24	1802	1848	2056
26	1785	1830	2034
28	1765	1804	2008
30	1750	1781	1980

6. Thermochemical Parameters:

Thermochemical Parameters for CH_2CH_2OH, CH_3CHOH, CH_3CH_2O, CH_2CHOH, CH_3CO, CH_2COH, and CHCHOH

	$H_{f,298}$	S_{298}	$C_{P,300}$	$C_{P,400}$	$C_{P,500}$	$C_{P,600}$	$C_{P,800}$	$C_{P,1000}$	$C_{P,1500}$
CH_2CH_2OH	-5.8	69.4	16.8	19.5	22.0	24.1	27.6	30.3	34.8
CH_3CHOH	-12.9	68.1	15.8	18.8	21.5	23.8	27.6	30.4	34.9
CH_3CH_2O	-2.7	66.8	15.8	18.8	21.7	24.1	28.2	31.2	36.0
CH_2CHOH	-29.1	62.2	15.0	18.1	20.5	22.5	25.5	27.6	31.1
CH_3CO	-2.0	63.7	12.1	14.1	16.1	17.8	20.7	22.8	26.2
CH_2COH	28.5	64.1	14.4	16.9	18.7	20.2	22.3	23.9	26.5
CHCHOH	32.2	62.8	14.7	17.7	20.0	21.6	23.6	24.9	27.0

Units of enthalpy are kcal mol^{-1}

Units of entropy and heat capacity are cal mol^{-1} K^{-1}

7. Experimental Mole Fraction Profiles:

a) Flame 1

	H2	CH3	CH4	H2O	C2H2	C2H3	C2H4	CO	C2H5	CH2O	C2H6	CH3O	CH3OH	O2	C3H3	aC3H4	pC3H4	Ar	C3H5	C3H6
0	0.16	5.05E-04	0.00235	0.083	0.00142	2.57E-05	0.00329	0.035	1.95E-05	0.00216	0.00301	6.29E-05	5.06E-04	0.23	4.60E-06	4.37E-06	1.64E-05	0.52	1.01E-05	1.24E-03
0.25	0.16042	4.50E-04	0.00236	0.0839	0.00144	1.66E-05	0.00334	0.03543	1.92E-05	0.0022	0.00305	3.21E-05	1.92E-04	0.23197	5.13E-06	8.79E-06	1.22E-05	0.51743	1.62E-05	9.49E-04
0.5	0.15967	5.75E-04	0.00255	0.0893	0.00152	6.20E-06	0.00371	0.03746	2.02E-05	0.00242	0.00291	2.00E-05	2.46E-04	0.22695	-5.08E-07	9.00E-06	1.09E-05	0.50644	1.10E-05	1.04E-03
0.75	0.15513	7.51E-04	0.00261	0.09437	0.00155	1.47E-05	0.0037	0.03753	2.93E-05	0.00241	0.00292	1.38E-05	3.02E-04	0.21657	1.02E-06	8.89E-06	1.98E-05	0.50179	1.75E-06	1.11E-03
1	0.15093	9.46E-04	0.00269	0.10097	0.00164	2.54E-05	0.00391	0.03846	2.47E-05	0.00237	0.00293	7.99E-06	1.84E-04	0.20631	4.10E-06	6.05E-06	1.76E-05	0.49496	5.05E-06	1.18E-03
1.25	0.14538	0.0012	0.00288	0.10781	0.00176	8.28E-06	0.00426	0.04041	2.85E-05	0.00256	0.00291	2.09E-05	1.87E-04	0.19562	1.65E-06	9.72E-06	1.85E-05	0.48891	5.30E-06	1.31E-03
1.5	0.14637	0.00135	0.00313	0.11489	0.00192	7.97E-06	0.00441	0.04252	4.06E-05	0.00247	0.00299	3.96E-05	2.66E-04	0.18706	-4.51E-06	7.55E-06	2.02E-05	0.48482	2.34E-05	1.26E-03
1.75	0.15341	0.00176	0.0034	0.11494	0.00225	3.56E-05	0.00546	0.0452	5.25E-05	0.00286	0.00316	1.42E-04	2.10E-04	0.19041	-7.29E-06	1.27E-05	2.73E-05	0.47573	2.96E-05	1.49E-03
2	0.14106	0.002	0.00358	0.13059	0.00233	2.98E-05	0.00531	0.04509	5.99E-05	0.0025	0.0031	5.58E-05	1.39E-04	0.17216	5.08E-06	2.80E-05	2.60E-05	0.47021	3.52E-05	1.67E-03
2.25	0.14867	0.00236	0.00402	0.13036	0.00266	4.84E-05	0.00582	0.05082	7.05E-05	0.00255	0.00291	9.40E-05	2.13E-04	0.17074	7.49E-06	2.46E-05	4.02E-05	0.46558	3.49E-05	1.74E-03
2.5	0.14751	0.00221	0.00426	0.1391	0.00285	3.45E-05	0.0061	0.05289	3.82E-05	0.00246	0.00262	1.02E-04	1.75E-04	0.16023	1.41E-05	2.95E-05	4.25E-05	0.46226	2.72E-05	1.50E-03
2.75	0.1419	0.00223	0.00441	0.14946	0.003	2.17E-05	0.00615	0.0534	2.30E-05	0.00214	0.00247	1.02E-04	2.15E-04	0.14351	1.12E-05	2.76E-05	4.93E-05	0.46013	3.54E-05	1.36E-03
3	0.13965	0.00234	0.00479	0.15578	0.00327	3.69E-05	0.00629	0.05864	3.65E-05	0.00204	0.00211	1.23E-04	1.13E-04	0.13729	2.27E-05	2.56E-05	6.85E-05	0.45671	3.57E-05	1.40E-03
3.25	0.1427	0.00188	0.00489	0.1619	0.00351	9.75E-06	0.00601	0.06461	2.14E-05	0.00176	0.00165	4.89E-05	1.37E-04	0.12881	1.78E-05	4.04E-05	5.75E-05	0.4535	4.22E-05	1.16E-03
3.5	0.13456	0.00187	0.00477	0.17401	0.00362	7.50E-06	0.00547	0.06641	1.34E-05	0.00138	0.00144	-1.06E-05	5.28E-05	0.11777	1.51E-05	3.28E-05	6.95E-05	0.44998	3.31E-05	1.11E-03
3.75	0.13118	0.0013	0.00457	0.18182	0.0037	2.47E-05	0.00486	0.07168	7.11E-06	0.00109	9.40E-04	1.87E-06	-1.40E-05	0.10791	0.00E+00	2.99E-05	6.03E-05	0.44668	1.27E-05	6.19E-04
4	0.1314	0.00104	0.00406	0.18826	0.00371	1.31E-05	0.00415	0.07559	2.33E-06	7.68E-04	6.64E-04	-7.87E-06	1.47E-04	0.10032	3.54E-06	1.06E-05	5.93E-05	0.44505	4.54E-06	4.36E-04
4.25	0.12875	7.22E-04	0.00357	0.19449	0.00364	1.14E-05	0.0034	0.08093	5.41E-06	6.99E-04	4.09E-04	3.53E-05	1.91E-04	0.0921	-2.12E-06	2.11E-05	3.44E-05	0.4429	1.39E-05	3.19E-04
4.5	0.12224	5.17E-04	0.0031	0.19996	0.00341	0	0.00272	0.08585	4.97E-06	4.40E-04	3.72E-04	4.41E-05	1.45E-04	0.08375	6.79E-07	2.11E-05	3.31E-05	0.44226	-7.41E-07	2.39E-04
4.75	0.12019	3.77E-04	0.00262	0.20762	0.00317	1.42E-05	0.00199	0.0892	7.75E-06	4.19E-04	1.84E-04	-1.02E-05	1.28E-04	0.07625	-1.34E-06	7.34E-06	3.47E-05	0.44095	7.40E-06	1.55E-04
5	0.12011	3.03E-04	0.0021	0.20989	0.00291	-2.07E-05	0.00152	0.09079	5.84E-06	3.16E-04	1.26E-05	6.41E-05	9.42E-05	0.06875	-1.23E-06	1.59E-05	2.61E-05	0.4424	-6.10E-06	1.71E-04
6	0.10846	6.36E-05	8.92E-04	0.23687	0.0018	1.46E-05	3.91E-04	0.09781	5.06E-06	1.08E-04	-2.38E-05	3.32E-05	1.19E-05	0.04614	1.87E-06	1.92E-06	2.61E-07	0.43627	5.94E-06	5.99E-05
7	0.10526	2.61E-05	3.43E-04	0.24879	9.38E-04	5.35E-06	1.20E-04	0.09929	1.14E-06	-1.96E-06	4.91E-05	6.25E-05	5.85E-05	0.02995	-3.41E-06	3.44E-06	9.07E-07	0.43525	5.26E-06	1.21E-05
8	0.0912	3.12E-05	1.90E-04	0.26512	4.29E-04	1.92E-05	1.71E-05	0.09542		3.30E-05	1.33E-05			0.01981	-4.19E-06	-1.13E-05	-1.27E-06	0.43777		1.03E-04
9	0.08896	-1.32E-05	6.99E-05	0.26493	2.00E-04	8.12E-06	1.43E-05	0.09322		2.36E-05	-1.86E-05			0.0127	4.14E-06		1.94E-07	0.4362		
10	0.0916	1.86E-05	2.55E-05	0.26623	1.01E-04	-3.43E-05	-8.89E-06	0.09168		8.45E-06	4.75E-06			0.00818				0.43629		
11	0.08296	4.26E-05	3.23E-05	0.27046	4.81E-05		5.03E-06	0.08677		5.74E-06	1.38E-06			0.00556				0.4378		
12	0.08803	4.78E-05	2.20E-05	0.26804	3.60E-05		3.15E-06	0.08526		3.59E-06	6.85E-06			0.00399				0.43934		
13	0.08677	4.75E-05	-3.76E-07	0.2691	2.23E-05		4.24E-06	0.08544		7.53E-06	3.42E-06			0.0028				0.4386		
14	0.08629	1.85E-05	5.01E-05	0.26247	1.39E-05		-5.50E-06	0.08629		2.23E-05	-1.81E-05			0.00184				0.44197		
15	0.0883	-1.69E-04	2.43E-05	0.26627	7.36E-06		-2.52E-05	0.08579		-1.73E-04	-4.85E-06			0.00137				0.43928		
18	0.0883	1.05E-04	7.79E-06	0.26844	1.04E-05		3.12E-05	0.08256		2.03E-05	-5.87E-06			5.05E-04				0.43991		
21	0.08971	7.84E-05	6.80E-05	0.27017	6.82E-06		-1.17E-05	0.08007		1.77E-05	-1.80E-06			1.51E-04				0.44051		
24	0.08915	3.78E-06	5.47E-06	0.26534	2.19E-07		3.75E-07	0.07689		-5.71E-07	-1.45E-06			-6.16E-05				0.44473		
27	0.09145	-1.31E-05	3.47E-05	0.26666	2.29E-06		7.80E-06	0.07502		9.88E-07	1.01E-05			1.65E-04				0.4465		
30	0.09123	1.54E-04	-1.16E-04	0.26721	1.34E-05		2.29E-05	0.07507		6.39E-05	1.94E-05			8.41E-05				0.45		

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	C3H7	CH2CHOH	CH3CHO	CO2	C2H5OH	C4H2	C4H4	13C4H6	C4H7	1C4H8	2C4H8	C4H9	Acetone	Propenols	Propanal	C4H10	CH3CHCHC	Butenols	Butanal	nButanol
0	5.81E-05	2.19E-04	1.05E-03	0.006	2.09E-04	-3.69E-07	3.43E-08	5.78E-05	1.53E-06	1.65E-04	1.01E-04	8.79E-06	1.82E-05	3.38E-05	9.24E-06		2.81E-04	2.73E-04		0.035
0.25	3.23E-05	1.73E-04	7.08E-04	0.00612	1.03E-04	-1.89E-06	3.66E-07	4.10E-05	3.99E-06	1.41E-04	1.23E-04	7.84E-06	3.74E-05	1.70E-05	-1.99E-05	3.44E-05	1.97E-04	1.92E-04	1.20E-03	0.03495
0.5	3.73E-05	2.15E-04	7.00E-04	0.00653	1.17E-04	1.06E-06	-6.85E-08	4.85E-05	2.83E-06	1.46E-04	1.02E-04	5.93E-06	2.19E-05	3.02E-05	-5.50E-06	7.97E-06	2.48E-04	2.40E-04	1.15E-03	0.03389
0.75	4.31E-05	2.33E-04	9.10E-04	0.00665	1.02E-04	0	-2.45E-07	4.51E-05	-1.38E-06	1.61E-04	1.33E-04	9.51E-06	8.07E-06	1.68E-05	-2.06E-05	-2.86E-05	2.11E-04	1.91E-04	1.25E-03	0.02971
1	3.58E-05	2.26E-04	8.38E-04	0.00653	1.15E-04	-3.99E-06	1.31E-06	6.35E-05	1.41E-06	1.56E-04	1.33E-04	1.22E-05	6.41E-05	1.16E-05	-4.35E-05	3.29E-05	2.54E-04	2.88E-04	1.23E-03	0.0262
1.25	4.00E-05	2.90E-04	9.70E-04	0.00704	5.50E-05	-5.70E-06	1.48E-06	7.58E-05	7.53E-07	2.07E-04	4.33E-05	9.72E-06	5.78E-05	1.48E-05	-3.06E-05	-3.90E-05	2.35E-04	2.25E-04	1.15E-03	0.02298
1.5	4.21E-05	2.54E-04	8.27E-04	0.00754	7.88E-05	3.80E-06	0.00E+00	6.42E-05	7.52E-07	2.15E-04	6.25E-05	7.44E-07	3.28E-05	1.34E-05	-2.72E-05	-3.32E-07	2.00E-04	1.81E-04	1.09E-03	0.0192
1.75	3.38E-05	2.82E-04	9.85E-04	0.00867	3.49E-05	-5.67E-06	1.59E-06	8.63E-05	5.63E-06	2.30E-04	1.03E-04	7.06E-06	6.93E-05	9.60E-07	-2.63E-05	7.55E-05	1.90E-04	1.72E-04	9.96E-04	0.0214
2	3.88E-05	2.89E-04	1.04E-03	0.00908	8.14E-05	-7.73E-06	6.60E-06	1.06E-04	5.58E-06	2.52E-04	5.02E-05	1.41E-05	5.23E-05	9.91E-07	2.38E-05	2.53E-05	1.91E-04	1.48E-04	9.13E-04	0.01296
2.25	2.70E-05	2.53E-04	1.10E-03	0.00967	5.61E-05	-4.10E-06	3.16E-06	1.74E-04	7.16E-06	1.97E-04	7.58E-05	1.06E-05	8.34E-05	2.71E-06	-3.14E-05	9.42E-05	2.64E-04	1.51E-04	7.49E-04	0.01464
2.5	1.57E-05	2.14E-04	9.94E-04	0.01013	1.09E-04	-4.48E-06	4.94E-06	1.77E-04	6.44E-06	1.96E-04	8.29E-05	1.13E-05	3.30E-05	1.09E-05	3.74E-05	8.39E-05	2.35E-04	1.58E-04	4.42E-04	0.01015
2.75	5.60E-06	1.21E-04	8.49E-04	0.01109	2.22E-06	2.51E-06	3.83E-06	1.74E-04	4.61E-06	1.65E-04	7.18E-05	8.07E-06	1.47E-05	1.25E-05	2.45E-05	2.22E-05	1.69E-04	8.14E-05	3.42E-04	0.00527
3	2.02E-05	1.31E-04	8.06E-04	0.01196	-1.35E-05	-1.89E-06	5.69E-06	2.00E-04	2.35E-06	1.25E-04	9.58E-05	1.32E-05	3.06E-06	1.53E-05	1.92E-05	4.25E-05	1.51E-04	5.48E-05	3.14E-04	0.00287
3.25	3.02E-05	7.99E-05	5.70E-04	0.0127	2.05E-05	1.01E-05	9.94E-06	1.54E-04	2.35E-06	6.56E-05	8.50E-05	9.64E-06	-6.29E-06	1.18E-05	3.76E-05	5.26E-05	9.26E-05	4.66E-05	1.65E-04	0.00241
3.5	1.66E-05	7.05E-05	6.74E-04	0.01386	6.31E-05	1.21E-05	9.12E-06	1.18E-04	1.64E-06	9.28E-05	1.28E-05	6.42E-07	1.99E-05	-1.41E-06	3.99E-05	6.64E-05	1.85E-05	1.11E-05	1.14E-04	2.98E-04
3.75	5.95E-06	1.61E-05	3.70E-04	0.01517	3.62E-05	9.66E-06	8.27E-06	1.17E-04	2.09E-06	1.67E-05	4.04E-05	4.60E-06	1.51E-05	0.00E+00	2.16E-05	2.82E-05	2.01E-05	7.35E-06	4.65E-05	-4.77E-05
4	-2.00E-06	2.63E-05	1.76E-04	0.0157	2.64E-05	8.72E-06	6.63E-06	7.60E-05	2.05E-06	1.90E-05	2.03E-05	9.75E-08	1.72E-05	-1.73E-06	-2.06E-05	2.30E-05	2.17E-05	4.45E-06	3.45E-05	9.62E-05
4.25	4.38E-06	-6.39E-06	1.58E-04	0.01674	-5.85E-06	2.23E-06	8.14E-06	3.56E-05	-8.17E-07	1.67E-05	-2.12E-06	2.37E-07	5.71E-06	-1.28E-06	-3.57E-06	1.87E-05	2.15E-05	4.23E-07	1.59E-05	5.84E-04
4.5	3.93E-06	7.26E-06	1.23E-04	0.01759	0	6.10E-06	4.77E-06	2.05E-05	2.10E-06	-2.62E-06	9.90E-06	-1.21E-06	-5.52E-06	6.38E-07	5.75E-06	6.12E-06	2.01E-05	-1.72E-06	1.43E-05	9.76E-05
4.75	-1.52E-06	1.54E-05	1.31E-04	0.01873	1.91E-05	4.99E-06	3.47E-06	2.33E-05	0.00E+00	3.97E-06	4.85E-06	1.30E-06	-9.92E-06	5.44E-06	2.41E-05	-3.04E-06	1.91E-05	9.77E-07	6.92E-06	3.27E-05
5	2.94E-07	8.27E-06	1.69E-04	0.01921	4.51E-05	3.68E-06	3.31E-06	2.57E-05	2.47E-06	2.76E-06		4.37E-06			6.14E-09	1.15E-06	3.69E-05	1.35E-06	3.31E-06	3.41E-04
6	5.35E-06	1.36E-05	6.09E-05	0.02389	1.06E-05	3.53E-07	-4.70E-07		3.34E-06			-1.04E-06			2.25E-06	-7.46E-06	-7.37E-06	-3.40E-06	1.56E-05	-4.36E-04
7	8.07E-07	9.06E-06	-1.75E-04	0.02688	-5.83E-05	-2.77E-06	-9.76E-07		5.99E-07			-9.38E-06			-4.64E-06	-3.35E-06	-7.27E-05	-1.49E-05	2.32E-06	-1.86E-04
8	1.29E-06	-1.19E-04	-2.89E-05	0.03037	-2.32E-06	1.71E-06	-3.08E-07					4.94E-06				5.20E-06		4.45E-06	2.04E-05	-2.16E-04
9				0.03434	1.97E-06	1.76E-07	7.93E-07									4.65E-06				-3.36E-04
10				0.03678	-8.31E-06	1.56E-06	7.88E-07													-4.36E-04
11				0.04032																8.32E-05
12				0.04157																8.25E-05
13				0.04306																1.49E-04
14				0.04249																1.63E-04
15				0.04488																6.60E-05
18				0.04852																2.47E-04
21				0.05069																3.61E-04
24				0.0521																1.45E-04
27				0.05321																2.07E-04
30				0.05446																7.52E-04

b) Flame 2

	H2	CH3	CH4	H2O	C2H2	C2H3	C2H4	CO	C2H5	CH2O	C2H6	CH3O	CH3OH	O2	C3H3	aC3H4	pC3H4	Ar	C3H5	C3H6
0	0.015	1.57E-04	0.00125	0.06	0.00166	-3.86E-05	0.00363	0.031	1.63E-05	0.00259	0.00188	1.64E-04	3.08E-05	0.09		-2.68E-06	3.29E-05	0.73	4.04E-06	1.27E-03
0.25	0.01531	5.44E-05	0.00126	0.06564	0.00166	3.71E-06	0.00368	0.03178	4.53E-06	7.48E-04	0.00191	1.20E-04	3.80E-05	0.09046	3.40E-06	3.82E-06	7.55E-06	0.731	2.35E-06	3.48E-04
0.5	0.01518	1.09E-04	0.00119	0.06418	0.00167	-2.68E-06	0.00347	0.03246	9.39E-06	0.00151	0.00183	8.78E-05	3.09E-05	0.08877	2.99E-06	5.20E-06	1.59E-05	0.72892	3.29E-06	7.82E-04
0.75	0.01541	2.20E-04	0.00118	0.06679	0.00167	0.00E+00	0.00369	0.03293	1.64E-05	0.00174	0.00181	1.24E-04	4.46E-05	0.08723	-3.03E-06	8.10E-06	1.94E-05	0.72751	-1.52E-06	9.07E-04
1	0.01614	2.80E-04	0.00123	0.06973	0.00171	-8.51E-06	0.00374	0.03252	1.85E-05	0.00159	0.00191	4.92E-05	-1.31E-05	0.08504	-1.53E-05	1.09E-05	1.65E-05	0.72486	3.54E-06	7.89E-04
1.25	0.01712	4.51E-04	0.00133	0.07254	0.00188	4.30E-05	0.00408	0.03473	2.01E-05	0.00221	0.00191	7.03E-05	4.14E-05	0.08277	2.90E-05	1.26E-05	3.09E-05	0.72291	1.30E-06	1.14E-03
1.5	0.0168	4.96E-04	0.00137	0.07417	0.00193	3.34E-05	0.00415	0.03568	2.10E-05	0.00181	0.00181	7.32E-05	5.44E-06	0.0792	-2.03E-05	6.86E-06	3.21E-05	0.71981	2.56E-06	9.47E-04
1.75	0.01879	6.13E-04	0.00146	0.07822	0.00207	1.52E-05	0.00447	0.03875	4.00E-05	0.00201	0.00187	5.67E-05	1.54E-05	0.07815	5.73E-06	1.62E-05	2.80E-05	0.71933	1.63E-05	1.05E-03
2	0.01904	7.60E-04	0.00149	0.08093	0.00218	1.34E-05	0.00457	0.03951	3.96E-05	0.00208	0.00191	3.09E-05	7.24E-05	0.0746	-1.18E-05	1.55E-05	3.49E-05	0.71671	1.49E-05	1.03E-03
2.25	0.01906	8.59E-04	0.00152	0.08393	0.0023	3.71E-05	0.00473	0.04052	4.38E-05	0.00211	0.00183	8.19E-05	1.08E-04	0.07057	3.79E-06	1.73E-05	4.16E-05	0.71535	1.95E-05	1.15E-03
2.5	0.01939	0.00101	0.00159	0.08675	0.00248	1.44E-05	0.00508	0.04218	5.72E-05	0.00228	0.00173	4.46E-05	1.09E-04	0.0669	8.62E-06	1.60E-05	4.26E-05	0.71384	3.25E-05	1.16E-03
2.75	0.0211	0.00115	0.0017	0.0912	0.00266	4.23E-05	0.00512	0.04462	4.56E-05	0.00228	0.00167	6.08E-05	8.82E-05	0.06397	8.57E-06	4.70E-06	5.62E-05	0.71311	2.63E-05	1.24E-03
3	0.0224	0.00126	0.00182	0.09276	0.00287	5.68E-05	0.00523	0.04631	4.06E-05	0.00191	0.00167	-1.14E-07	1.59E-04	0.05922	1.69E-05	2.89E-05	4.39E-05	0.71101	4.43E-05	1.03E-03
3.25	0.02255	0.00155	0.0019	0.09811	0.00311	4.94E-05	0.0058	0.04961	2.35E-05	0.00203	0.00141	3.55E-07	8.49E-05	0.05632	1.27E-05	3.28E-05	5.99E-05	0.71014	3.51E-05	1.16E-03
3.5	0.0222	0.00133	0.00191	0.10188	0.00317	-2.39E-06	0.00539	0.05325	3.35E-05	0.00175	0.00116	-6.07E-05	6.30E-05	0.05189	2.87E-05	3.46E-05	5.36E-05	0.70935	3.37E-05	9.89E-04
3.75	0.02303	0.00137	0.00192	0.10374	0.00338	1.71E-05	0.00528	0.05685	3.45E-05	0.0016	9.53E-04	1.17E-04	3.32E-05	0.04753	2.14E-05	2.80E-05	7.84E-05	0.70787	4.41E-05	9.66E-04
4	0.02319	0.00113	0.00203	0.10613	0.00354	3.76E-05	0.00477	0.05832	1.71E-05	0.00124	6.08E-04	-3.24E-05	9.16E-05	0.04324	4.12E-05	3.52E-05	7.23E-05	0.707	3.50E-05	7.78E-04
4.25	0.02395	8.37E-04	0.00199	0.11149	0.00363	-2.40E-06	0.00413	0.06444	1.70E-05	8.88E-04	5.48E-04	3.88E-06	9.88E-06	0.0401	7.37E-06	1.70E-05	6.38E-05	0.70617	3.15E-05	4.86E-04
4.5	0.02313	4.28E-04	0.00191	0.11404	0.00361	1.40E-05	0.00322	0.06835	-1.05E-06	5.19E-04	4.02E-04	-1.08E-04	-2.53E-05	0.03574	1.83E-05	2.40E-05	4.02E-05	0.70516	1.16E-05	2.17E-04
4.75	0.02372	3.65E-04	0.0015	0.11895	0.00344	7.47E-06	0.00249	0.07456	1.90E-06	5.61E-04	9.25E-05	-5.13E-05	-4.35E-05	0.03253	-9.23E-06	3.45E-05	3.86E-05	0.70497	1.81E-05	1.51E-04
5	0.02433	1.62E-04	0.00125	0.12134	0.00307	-1.99E-06	0.00158	0.07832	7.02E-06	3.05E-04	7.29E-05	2.70E-05	1.68E-05	0.02893	-1.63E-05	2.37E-05	2.53E-05	0.70485	5.22E-06	9.51E-05
6	0.02119	5.10E-05	2.51E-04	0.12965	0.00126	2.35E-05	2.23E-04	0.07967	3.53E-06		8.03E-05	3.91E-05	1.52E-05	0.01744	1.24E-05	5.97E-06		0.70402	1.26E-05	0.00E+00
7	0.01887	-2.98E-06	4.19E-05	0.13385	2.68E-04	2.74E-06	4.21E-05	0.07331	2.64E-07		7.35E-06	-1.03E-05	3.61E-06	0.01199	9.33E-07	-5.39E-06		0.70463	-1.14E-07	-5.49E-06
8	0.01801	3.15E-05	1.46E-05	0.13733	7.95E-05	-3.87E-05	-5.31E-06	0.06933	9.79E-06		1.16E-05	-9.83E-06	-8.58E-06	0.00934	3.94E-06	2.28E-05		0.70498	-6.36E-05	0.00E+00
9	0.01841	1.33E-05	1.15E-05	0.13589	2.89E-05	2.04E-06	0.00E+00	0.06441			1.73E-05	-1.20E-05	-1.84E-06	0.00711	-4.16E-06			0.70361		
10	0.01719	-2.62E-07		0.13178	1.71E-06	-3.57E-08	1.27E-06	0.05898			2.59E-08	-6.67E-08	7.35E-07	0.00612	2.93E-09			0.70498		
11	0.01738	8.14E-07		0.13185	3.54E-06			0.05538			-3.87E-06	1.62E-07	8.83E-07	0.00551	0.00E+00			0.7056		
12	0.01755	1.06E-05		0.13326	1.71E-06			0.05506			3.10E-06	-6.14E-07	8.45E-07	0.0045	-1.95E-07			0.70524		
13	0.01748			0.13075	-5.84E-06			0.05135			-3.39E-06	1.61E-05	4.44E-05	0.00481	1.85E-05			0.70614		
14	0.0162			0.12919	-6.60E-06			0.04814			3.03E-06	2.02E-06	6.85E-06	0.00488	1.50E-05			0.70572		
15	0.01838			0.12934	3.17E-06			0.05007			2.35E-06	3.48E-06	-6.64E-05	0.00367	-2.57E-05			0.70508		
18	0.01873			0.13132	6.41E-06			0.0483			8.45E-06	-2.39E-05	-8.75E-05	3.02E-03	-3.14E-05			0.70694		
21	0.01978			0.12949	4.53E-06			0.04794			5.54E-06	-3.76E-06	-7.12E-05	2.32E-03	-1.17E-05			0.7085		
24	0.02024			0.12904	6.19E-06			0.04685			3.17E-06	-1.88E-06	5.55E-07	1.97E-03	-2.02E-07			0.70866		
27	0.01994			0.12922	3.51E-06			0.04524			-1.92E-06	9.94E-07	3.91E-06	1.58E-03	-2.70E-06			0.70818		
30	0.02077			0.1278	2.87E-05			0.04536			-1.99E-05	-1.08E-04	-2.29E-04	1.11E-03	-2.29E-05			0.71		

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	C3H7	CH2CHOH	CH3CHO	CO2	C2H5OH	C4H2	C4H4	13C4H6	C4H7	1C4H8	2C4H8	C4H9	Acetone	Propenols	Propanal	C4H10	CH3CHCHC	Butenols	Butanal	nButanol
0	3.60E-05	3.46E-04	7.00E-04	0.019	1.43E-04	-1.32E-06	1.45E-06	1.01E-04	1.01E-05	2.46E-04	7.70E-05	1.10E-04	4.81E-05		1.19E-04	1.51E-04	3.81E-04	1.24E-04	6.34E-04	0.023
0.25	7.76E-06	1.15E-04	2.14E-04	0.01954	2.67E-05	1.98E-06	1.86E-06	2.83E-05	-6.19E-07	8.04E-05	1.76E-05	2.58E-05	1.35E-05		3.76E-05	4.79E-05	1.02E-04	3.54E-05	1.95E-04	0.02318
0.5	8.81E-06	2.14E-04	4.52E-04	0.01979	6.31E-05	-1.89E-06	8.85E-07	3.98E-05	-1.83E-06	1.19E-04	2.85E-05	3.21E-05	1.14E-05		4.89E-05	6.28E-05	1.89E-04	5.70E-05	3.81E-04	0.02174
0.75	2.18E-05	3.81E-04	5.16E-04	0.02056	3.35E-05	4.16E-06	5.02E-06	7.60E-05	-3.72E-06	2.16E-04	4.73E-05	2.69E-05	2.61E-05		9.06E-05	8.57E-05	2.82E-04	8.33E-05	4.41E-04	0.02042
1	1.43E-05	3.62E-04	6.22E-04	0.02159	7.42E-05	-1.70E-06	5.20E-06	8.59E-05	-2.29E-06	1.91E-04	5.71E-05	-1.43E-05	2.70E-05		1.21E-04	2.57E-05	2.60E-04	8.27E-05	3.53E-04	0.01902
1.25	2.78E-05	3.06E-04	9.45E-04	0.02171	1.28E-04	-5.45E-07	4.53E-06	7.43E-05	1.78E-06	2.43E-04	3.72E-05	4.06E-05	2.24E-05		1.01E-04	-3.91E-06	2.18E-04	5.87E-05	5.15E-04	0.0187
1.5	3.08E-05	4.12E-04	6.44E-04	0.0223	7.72E-05	2.82E-06	3.12E-06	9.62E-05	2.01E-06	2.21E-04	4.95E-05	4.62E-06	1.67E-05		9.67E-05	5.78E-05	3.09E-04	8.15E-05	3.98E-04	0.0163
1.75	2.12E-05	3.86E-04	7.10E-04	0.02282	9.43E-05	-3.11E-06	1.56E-07	8.95E-05	3.53E-06	2.12E-04	3.17E-05	4.43E-05	2.22E-05		1.08E-04	2.90E-05	2.57E-04	6.48E-05	4.42E-04	0.01555
2	1.08E-05	3.65E-04	8.10E-04	0.02362	8.47E-05	-1.91E-06	6.74E-06	1.00E-04	4.74E-06	2.14E-04	4.87E-05	1.08E-06	2.15E-05		1.07E-04	-1.09E-05	1.90E-04	4.93E-05	3.55E-04	0.01362
2.25	1.77E-05	3.69E-04	7.21E-04	0.02414	1.09E-04	-2.41E-06	5.66E-06	1.29E-04	4.53E-06	2.15E-04	4.94E-05	5.48E-05	4.64E-06		7.83E-05	5.48E-05	2.55E-04	3.92E-05	3.67E-04	0.01121
2.5	2.73E-05	3.33E-04	7.62E-04	0.02521	6.74E-05	5.24E-06	2.36E-06	1.32E-04	3.86E-06	2.45E-04	4.23E-05	-2.72E-06	1.13E-05		1.18E-04	-1.86E-05	1.78E-04	4.60E-05	3.46E-04	0.01034
2.75	-1.00E-06	2.21E-04	8.10E-04	0.02617	5.99E-05	1.52E-06	6.82E-06	1.54E-04	3.75E-06	2.43E-04	4.21E-05	-1.06E-05	2.17E-05		4.43E-05	1.66E-05	1.43E-04	1.79E-05	3.06E-04	0.00872
3	2.23E-05	2.60E-04	8.34E-04	0.02559	1.44E-05	3.71E-06	9.12E-06	1.53E-04	4.55E-06	1.94E-04	3.96E-05	2.32E-05	6.64E-06		4.80E-05	3.12E-05	1.98E-04	1.62E-05	2.23E-04	0.00717
3.25	-1.06E-07	1.52E-04	8.82E-04	0.02681	6.89E-05	7.58E-06	1.09E-05	1.88E-04	-1.84E-06	1.99E-04	4.94E-05	2.00E-05	2.49E-06		5.60E-05	5.40E-05	8.60E-05	1.35E-05	1.94E-04	0.00501
3.5	-1.02E-06	1.23E-04	7.14E-04	0.02808	8.80E-05	3.83E-06	1.34E-05	1.92E-04	-2.37E-06	1.66E-04	2.48E-05	4.53E-05	1.10E-06		6.01E-05	-1.58E-05	7.33E-05	3.66E-06	1.20E-04	3.14E-03
3.75	-2.56E-06	7.72E-05	7.44E-04	0.02871	2.78E-05	2.17E-06	1.13E-05	1.92E-04	1.29E-06	9.98E-05	3.61E-05	9.02E-06	3.62E-06		5.54E-05	-3.72E-05	4.99E-05	2.88E-06	7.45E-05	1.64E-03
4	9.25E-06	2.94E-05	4.94E-04	0.02941	-1.43E-05	1.45E-05	1.47E-05	1.89E-04	-1.05E-06	7.61E-05	1.85E-05	-9.71E-06	1.05E-05		3.06E-05	2.21E-05	3.90E-05	2.36E-06	6.52E-05	5.63E-04
4.25	1.30E-06	2.15E-05	3.28E-04	0.03062	-3.09E-05	1.11E-05	1.78E-05	1.98E-04	9.69E-07	4.38E-05	2.00E-05	6.37E-06	7.38E-06		2.18E-05	-3.36E-06	2.90E-05	3.91E-07	1.74E-05	6.25E-04
4.5	-3.74E-06	1.57E-05	1.41E-04	0.03204	-1.11E-05	5.55E-06	1.30E-05	8.65E-05	-9.22E-07	2.67E-06	1.22E-05	3.38E-06	3.20E-06		3.32E-06	4.24E-06	4.19E-06	-5.11E-07	1.53E-05	0.00E+00
4.75	-8.31E-06	1.89E-05	1.13E-04	0.03388	-6.85E-06	7.97E-06	1.18E-05	7.07E-05	-3.30E-07	1.02E-05	-2.24E-06	-9.17E-07	3.85E-06		2.68E-07	-8.51E-07	1.26E-05	6.11E-07	5.03E-06	-3.17E-04
5	-2.27E-05	8.33E-06	3.81E-05	0.03491	2.69E-05	9.35E-06	5.94E-06	2.97E-05		-1.23E-08	3.95E-05	-1.57E-06	2.04E-06		-3.96E-06	1.91E-07	4.00E-05	4.86E-07	3.09E-06	-9.31E-05
6	1.23E-05	2.78E-05	-2.26E-06	0.04272		-2.45E-07	-3.94E-07	1.74E-05		1.27E-05	7.70E-06		8.94E-07		-2.09E-05		3.87E-05	3.86E-06		-5.03E-04
7	1.19E-07	3.65E-07	-4.34E-06	0.05025	-7.97E-06	-6.87E-07	-1.10E-06	2.17E-07	8.63E-08	-1.10E-06	0.00E+00		1.34E-07		-4.19E-07		7.01E-07	1.72E-07		-3.39E-04
8	-4.78E-07		5.09E-05	0.05613	-2.81E-05	6.59E-07	-6.62E-07	1.61E-05		2.22E-05			-9.07E-05		1.58E-05		0.00E+00	2.03E-05		-1.91E-04
9				0.05913	7.90E-06	1.53E-06	-1.64E-06													-3.05E-04
10				0.061	-2.34E-07	7.55E-08	-9.71E-08													-1.67E-04
11				0.06381																
12				0.06595																
13				0.06727																
14				0.06856																
15				0.06816																
18				0.07048																
21				0.07051																
24				0.07058																
27				0.07191																
30				0.07144																

c) Flame 3

	H2	CH3	CH4	H2O	C2H2	C2H3	C2H4	CO	C2H5	CH2O	C2H6	CH3O	CH3OH	O2	C3H3	aC3H4	pC3H4	Ar	C3H5	C3H6
0	0.023	7.18E-04	0.00258	0.07	0.00245	5.90E-05	0.00808	0.035	4.13E-05	0.00553	0.00221	7.60E-05	6.43E-04	0.3	1.06E-05	2.32E-05	5.15E-05	0.44	1.81E-05	2.18E-03
0.25	0.02279	7.24E-04	0.00264	0.07002	0.00241	1.77E-05	0.00778	0.03646	3.06E-05	0.00539	0.0022	6.05E-05	6.35E-04	0.29857	6.11E-06	1.79E-05	5.15E-05	0.43963	1.52E-05	2.19E-03
0.5	0.0241	9.12E-04	0.00269	0.06936	0.00246	5.03E-05	0.00822	0.03865	3.34E-05	0.00575	0.00223	4.61E-05	6.29E-04	0.29119	6.10E-06	2.19E-05	6.04E-05	0.43535	1.58E-05	2.37E-03
0.75	0.02502	0.00121	0.00273	0.07254	0.00268	6.92E-05	0.00927	0.03986	5.15E-05	0.00647	0.00263	7.88E-05	6.24E-04	0.28706	2.32E-06	2.91E-05	8.65E-05	0.43048	2.96E-05	2.75E-03
1	0.02597	0.00127	0.00279	0.07222	0.00272	3.28E-05	0.00847	0.04348	4.99E-05	0.00546	0.00239	4.71E-05	5.50E-04	0.27674	1.26E-05	2.62E-05	6.31E-05	0.42653	2.52E-05	2.41E-03
1.25	0.02692	0.00171	0.00303	0.07683	0.00295	1.03E-04	0.00934	0.04465	7.14E-05	0.00632	0.00238	6.51E-05	6.31E-04	0.27119	9.33E-06	2.37E-05	7.39E-05	0.42209	3.23E-05	2.58E-03
1.5	0.02879	0.00219	0.00316	0.08231	0.00309	1.25E-04	0.01009	0.04759	9.42E-05	0.00672	0.00223	9.89E-05	6.21E-04	0.26422	3.42E-05	3.27E-05	8.77E-05	0.41775	5.05E-05	2.93E-03
1.75	0.0294	0.00252	0.00322	0.08644	0.00326	8.31E-05	0.01028	0.05201	1.08E-04	0.00655	0.00234	3.27E-05	5.55E-04	0.25249	2.89E-05	3.80E-05	9.01E-05	0.41464	6.27E-05	2.92E-03
2	0.03193	0.00308	0.00346	0.09427	0.00353	1.21E-04	0.01057	0.05509	1.10E-04	0.00661	0.00204	1.40E-05	5.72E-04	0.24265	3.58E-05	4.39E-05	9.58E-05	0.41041	6.45E-05	3.00E-03
2.25	0.03313	0.00355	0.00378	0.10067	0.00373	1.27E-04	0.01113	0.06029	1.36E-04	0.00671	0.00205	8.50E-05	5.41E-04	0.23255	5.30E-05	4.00E-05	9.84E-05	0.40723	8.41E-05	3.10E-03
2.5	0.03479	0.00423	0.00382	0.10946	0.00402	1.15E-04	0.01189	0.06662	1.34E-04	0.00695	0.00171	3.95E-05	5.12E-04	0.22307	5.02E-05	4.75E-05	1.09E-04	0.4039	1.12E-04	3.26E-03
2.75	0.0358	0.00426	0.00409	0.11511	0.00424	1.46E-04	0.01175	0.07226	1.12E-04	0.00613	0.00175	8.68E-05	4.70E-04	0.21015	4.81E-05	5.90E-05	9.68E-05	0.40163	1.13E-04	3.06E-03
3	0.0371	0.00419	0.0043	0.12588	0.0047	7.90E-05	0.01152	0.08035	9.92E-05	0.00549	0.00134	5.73E-05	3.52E-04	0.20369	5.47E-05	7.30E-05	1.39E-04	0.39838	1.30E-04	2.81E-03
3.25	0.03837	0.00408	0.0045	0.13564	0.00496	7.57E-05	0.0114	0.08592	7.63E-05	0.00497	0.00115	7.67E-05	2.82E-04	0.19092	5.98E-05	7.61E-05	1.31E-04	0.3966	1.27E-04	2.60E-03
3.5	0.04001	0.0035	0.00433	0.14429	0.00508	4.83E-05	0.01018	0.09683	3.58E-05	0.00428	7.72E-04	1.45E-04	1.65E-04	0.17771	6.60E-05	8.46E-05	1.47E-04	0.3948	1.08E-04	2.07E-03
3.75	0.04013	0.00265	0.00409	0.15345	0.00505	5.42E-05	0.00842	0.11057	2.33E-05	0.00331	4.81E-04	1.87E-05	2.35E-04	0.1658	4.12E-05	8.13E-05	1.50E-04	0.39306	6.89E-05	1.57E-03
4	0.04092	0.00189	0.00357	0.163	4.75E-03	2.53E-05	0.00659	0.11899	7.50E-06	0.00251	2.49E-04	-1.08E-05	1.68E-04	0.15487	2.54E-05	6.88E-05	1.27E-04	0.39159	3.87E-05	1.13E-03
4.25	0.03903	1.19E-03	0.00301	0.17249	4.37E-03	5.77E-06	0.0048	0.1325	1.00E-05	1.86E-03	1.79E-04	-3.45E-05	5.77E-05	0.14542	1.48E-05	6.67E-05	9.44E-05	0.3905	1.68E-05	7.64E-04
4.5	0.03779	7.07E-04	0.00238	0.18469	4.03E-03	3.37E-05	0.00347	0.1383	7.23E-06	1.48E-03	4.61E-05	-2.76E-05	6.68E-05	0.13464	6.39E-07	3.37E-05	5.93E-05	0.38958	4.14E-06	4.57E-04
4.75	0.03705	3.29E-04	0.00169	0.19178	3.31E-03	2.70E-05	0.00223	0.14422	4.90E-06	9.93E-04	1.10E-04	5.75E-06	8.35E-05	0.12591	3.16E-06	2.01E-05	2.36E-05	0.38926	3.57E-06	2.18E-04
5	0.03502	1.94E-04	0.00146	0.19573	2.67E-03	4.81E-06	0.00133	0.14298	3.22E-06	6.79E-04	-9.14E-06	-1.86E-05	3.44E-05	0.1217	0.00E+00	4.66E-06	9.89E-06	0.3891	3.59E-06	1.07E-04
5.5	0.03376	4.36E-05	7.05E-04	0.20635	1.57E-03	1.61E-05	4.66E-04	0.14882		2.73E-04	-2.04E-05	6.34E-06	1.06E-05	0.10886	-5.24E-07	1.67E-06	7.93E-07	0.38885		1.35E-05
6	0.03104	-7.38E-06	3.83E-04	0.21562	8.46E-04	9.97E-07	1.27E-04	0.145		7.92E-05	-1.70E-05	-6.61E-07	1.23E-05	0.10005	-3.23E-06	0.00E+00	5.53E-07	0.38883		-1.43E-06
6.5	0.0297	6.90E-06	2.08E-04	0.22086	4.68E-04	-2.49E-06	4.98E-05	0.13863		6.45E-05	-9.63E-06	1.65E-06	-4.46E-06	0.09349	5.40E-07	2.33E-05	-4.64E-06	0.38891		1.20E-06
7	0.0275	1.87E-06	1.57E-04	0.22471	2.56E-04	1.44E-06	2.62E-05	0.13459		2.64E-05	7.05E-06	2.39E-07	-1.50E-05	0.08861	-3.51E-06	7.90E-07	-1.21E-07	0.38878		
7.5	0.02683	-1.33E-05	6.82E-05	0.22352	1.21E-04	-9.70E-06	8.53E-06	0.12909		6.95E-06	2.17E-05	-2.23E-06	0.00E+00	0.08353	7.78E-07			0.38915		
8	0.02682	-1.14E-05	1.42E-04	0.23072	6.01E-05	0.00E+00	1.03E-05	0.12437		4.03E-06	2.21E-05	0.00E+00	6.05E-06	0.08021	-5.08E-07			0.38908		
10	0.02723	0.00E+00	7.54E-05	0.22836	1.36E-05	0.00E+00		0.11106				0.00E+00		0.07107				0.38975		
12	0.02742		9.83E-05	0.22892	1.53E-05			0.10102						0.06659				0.38984		
14	0.02827		2.26E-05	0.22412	-1.89E-06			0.0953						0.06431				0.39027		
16	0.02882		3.78E-05	0.2206	6.53E-06			0.09197						0.06122				0.39082		
18	0.02971		-1.34E-04	0.22379	1.83E-05			0.09002						5.89E-02				0.39099		
20	0.03011		3.64E-05	0.22253	-2.66E-06			0.0889						5.82E-02				0.39148		
22	0.03039		5.37E-05	0.22825	-4.54E-06			0.089						5.79E-02				0.3916		
24	0.03049		2.57E-05	0.23717	3.35E-06			0.08813						5.69E-02				0.39214		
26	0.03069		2.80E-06	0.23309	-9.92E-06			0.088						5.63E-02				0.39262		
28	0.03149		3.05E-05	0.23283	6.24E-07			0.08825						0.05513				0.3932		
30	0.03154			0.23723	1.70E-05			0.08862						0.05327				0.394		

	C3H7	CH2CHOH	CH3CHO	C3H8	CO2	C2H5OH	C4H2	C4H4	13C4H6	C4H7	1C4H8	2C4H8	C4H9	Acetone	Propenols	Propanal	C4H10	CH3CHCHC	Butenols	Butanal	nButanol
0	4.06E-05	2.67E-04	1.88E-03	1.53E-03	0.025	2.12E-04	4.71E-06	8.73E-06	4.75E-05	6.15E-06	5.48E-04	1.38E-04	1.74E-05	5.83E-05	-5.51E-06	2.44E-04	2.76E-04	1.89E-04	1.80E-04	1.17E-03	0.05
0.25	3.07E-05	2.51E-04	1.80E-03	1.50E-03	0.02471	1.86E-04	5.14E-06	6.53E-06	4.65E-05	4.13E-06	4.80E-04	1.16E-04	1.92E-05	4.60E-05	-4.29E-06	2.46E-04	2.18E-04	1.74E-04	1.40E-04	1.17E-03	0.04993
0.5	3.81E-05	3.29E-04	1.86E-03	1.49E-03	0.02508	2.30E-04	6.14E-06	3.76E-06	4.92E-05	6.44E-06	5.52E-04	1.01E-04	9.02E-06	4.32E-05	-3.27E-06	2.56E-04	1.52E-04	1.83E-04	1.64E-04	1.25E-03	0.04795
0.75	4.30E-05	4.15E-04	2.19E-03	1.63E-03	0.02606	2.27E-04	1.71E-06	8.29E-06	5.66E-05	4.32E-06	5.92E-04	1.33E-04	1.30E-05	6.42E-05	4.26E-06	2.56E-04	1.76E-04	2.11E-04	1.78E-04	1.39E-03	0.04332
1	3.75E-05	3.35E-04	1.84E-03	1.53E-03	0.02663	2.10E-04	3.50E-06	6.40E-06	5.28E-05	6.21E-06	5.70E-04	9.02E-05	2.07E-05	6.71E-05	7.53E-06	2.14E-04	1.30E-04	1.86E-04	1.57E-04	1.20E-03	0.03895
1.25	4.77E-05	4.01E-04	2.02E-03	1.60E-03	0.02759	1.78E-04	6.06E-07	7.87E-06	6.03E-05	5.81E-06	6.35E-04	9.91E-05	1.18E-05	7.64E-05	4.81E-06	2.36E-04	1.70E-04	1.85E-04	2.12E-04	1.23E-03	0.03895
1.5	5.50E-05	4.55E-04	2.20E-03	1.60E-03	0.02882	2.02E-04	1.68E-06	8.72E-06	7.10E-05	6.59E-06	7.28E-04	1.26E-04	1.45E-05	4.91E-05	1.80E-05	2.60E-04	1.75E-04	1.96E-04	1.94E-04	1.30E-03	0.0342
1.75	4.54E-05	4.42E-04	2.19E-03	1.60E-03	0.02964	1.80E-04	-3.69E-06	1.02E-05	7.59E-05	6.52E-06	6.69E-04	1.23E-04	2.10E-05	5.96E-05	1.27E-05	2.24E-04	1.95E-04	1.66E-04	1.50E-04	1.17E-03	0.02883
2	4.40E-05	4.27E-04	2.22E-03	1.53E-03	0.03087	8.63E-05	9.99E-06	9.28E-06	8.44E-05	6.08E-06	6.57E-04	9.74E-05	1.80E-05	3.24E-05	1.49E-05	2.25E-04	1.59E-04	1.58E-04	1.23E-04	1.06E-03	0.02914
2.25	4.28E-05	4.44E-04	2.22E-03	1.56E-03	0.03218	1.73E-04	8.18E-06	1.32E-05	9.58E-05	8.72E-06	6.95E-04	1.07E-04	4.41E-06	3.41E-05	1.22E-05	2.04E-04	1.23E-04	1.36E-04	1.15E-04	9.12E-04	0.02425
2.5	3.35E-05	4.17E-04	2.45E-03	1.24E-03	0.03392	7.76E-05	7.45E-06	1.86E-05	1.21E-04	9.35E-06	6.93E-04	1.02E-04	9.78E-06	2.78E-05	1.78E-05	1.86E-04	1.04E-04	1.15E-04	1.16E-04	8.11E-04	0.01577
2.75	1.35E-05	3.24E-04	2.19E-03	1.20E-03	0.03513	6.63E-05	2.03E-06	1.71E-05	1.22E-04	8.01E-06	5.41E-04	1.08E-04	-1.99E-06	3.11E-05	5.99E-06	1.36E-04	1.13E-04	9.55E-05	7.44E-05	5.79E-04	0.01254
3	1.70E-05	2.62E-04	1.98E-03	8.95E-04	0.03709	5.77E-05	1.00E-05	2.21E-05	1.27E-04	8.14E-06	4.46E-04	1.01E-04	1.05E-06	1.05E-05	1.59E-05	1.48E-04	9.36E-05	6.84E-05	5.54E-05	4.08E-04	0.00705
3.25	1.24E-05	1.95E-04	1.87E-03	8.08E-04	0.03914	6.21E-05	1.49E-05	2.68E-05	1.43E-04	7.02E-06	3.42E-04	7.92E-05	3.38E-06	2.28E-05	5.57E-06	7.45E-05	7.75E-05	4.48E-05	1.38E-05	2.95E-04	0.00506
3.5	8.25E-06	9.16E-05	1.40E-03	6.43E-04	0.04038	1.00E-04	1.00E-05	2.74E-05	1.18E-04	1.02E-05	1.97E-04	6.55E-05	-3.97E-06	1.82E-05	1.70E-06	4.77E-05	7.25E-05	3.21E-05	2.75E-05	1.81E-04	3.65E-03
3.75	5.34E-06	7.55E-05	9.72E-04	4.18E-04	0.04308	-3.22E-06	7.71E-06	2.99E-05	9.73E-05	2.84E-06	1.37E-04	5.59E-05	-4.86E-06	7.28E-06	3.51E-06	3.53E-05	9.63E-06	2.92E-05	3.99E-06	1.09E-04	2.22E-03
4	-1.04E-05	2.82E-05	6.61E-04	2.32E-04	0.04624	6.27E-06	8.51E-06	2.95E-05	6.87E-05	1.64E-06	5.76E-05	3.11E-05	3.87E-06	1.61E-05	2.43E-06	1.03E-05	-5.85E-06	1.68E-05	1.84E-05	5.12E-05	1.42E-04
4.25	-1.48E-06	1.33E-05	4.10E-04	1.32E-04	0.04825	1.90E-06	8.87E-06	2.23E-05	3.81E-05	3.29E-06	9.52E-06	2.13E-05	-4.25E-07	7.28E-06	-5.32E-06	2.41E-05	8.02E-06	7.54E-06	1.42E-05	2.38E-05	1.44E-04
4.5	5.22E-07	8.46E-06	1.94E-04	5.64E-05	0.05144	-4.45E-06	5.42E-06	1.48E-05	1.96E-05	5.51E-07	-3.69E-07	1.13E-05	-4.71E-06	9.75E-06	1.98E-06	-1.37E-05	1.61E-05	7.54E-06	1.10E-05	4.55E-06	-9.24E-04
4.75	-6.13E-07	3.35E-06	8.86E-05	3.33E-05	0.05395	-2.00E-05	5.35E-06	7.81E-06	8.30E-06	-4.96E-07	-7.12E-06	8.75E-06	3.48E-06	-1.36E-06	9.24E-06	-4.44E-07	1.03E-05	-1.01E-07	9.16E-06	3.16E-06	-7.82E-04
5	-9.70E-07	-1.34E-06	1.79E-05	2.99E-05	0.05686	-1.59E-05	3.61E-06	6.39E-06	2.92E-06	-4.93E-07	-1.35E-06	2.97E-06	4.87E-06	9.61E-07	5.22E-06	-9.21E-06	8.23E-06	-7.20E-07	-5.17E-06	3.68E-07	-4.41E-04
5.5			5.12E-06	1.76E-05	0.06261	-8.46E-06	2.70E-06	1.69E-06	4.73E-07	-1.42E-07			9.74E-07	-1.21E-08		1.13E-06	6.92E-06	-3.21E-06		9.14E-08	2.46E-04
6			-5.15E-07	1.11E-07	0.06747	2.14E-06	3.40E-07	8.21E-07	-3.55E-07	8.07E-08			-3.96E-07	0.00E+00		7.08E-07	6.32E-07	-1.74E-07		-3.59E-07	-4.92E-05
6.5			2.36E-06	5.75E-06	0.07218	-6.15E-07	1.99E-07	2.97E-07	3.15E-06				6.68E-07	-3.33E-07		6.65E-06	-9.63E-07	-8.19E-07		7.14E-06	2.95E-04
7			5.13E-07		0.07763	-9.53E-07	-2.16E-07										-1.52E-06				4.43E-04
7.5					0.08098		3.82E-07														-4.41E-04
8					0.08539		9.35E-08														0.00E+00
10					0.09782																-1.46E-04
12					0.10643																-3.88E-04
14					0.11201																-7.70E-04
16					0.11632																1.43E-04
18					0.11973																-3.81E-04
20					0.1215																8.51E-04
22					0.12398																7.55E-04
24					0.12626																5.62E-04
26					0.12809																4.65E-05
28					0.12921																1.38E-04
30					0.13119																-4.56E-05