

Supplementary Materials

**Global Minimum Profile Error (GMPE) - A Least-Squares-Based Approach
for Extracting Macroscopic Rate Coefficients for Complex Gas-phase
Chemical Reactions**

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Text S1: MSMC input for C₂H₂ + OH system

```
<Description>
Test case for C2H2 + OH
</Description>

<NodeNumber>
2
</NodeNumber>

<CoreNumber>
4
</CoreNumber>

<ArrhFitting>
modified
</ArrhFitting>

<PESprint>
on
</PESprint>

<nasafit>
off
</nasafit>

<caltst>
on
</caltst>

<debugmode>
on
</debugmode>

<Kinetics>
Profiles = none
Init = OH
NM = 1.0E-04
Omega= Lennard-Jones
BoltzmannReactant = on
Deter=(mpack, high)!! Deter for Determinestic method
Stoch=(msmc, boost, 1.0E6)!! Stoch for Stochastic method
</Kinetics>

<ELMT>
CBS-QB3
</ELMT>
```

<Precision>

256

</Precision>

<Temperature>!!Unit: K

300

400

500

600

700

800

900

1000

1100

1200

1300

1400

1500

1600

1700

1800

1900

2000

</Temperature>

<Pressure>!!Unit: torr

760

</Pressure>

<EnergyStep>!!Unit: cm⁻¹

200

</EnergyStep>

<Collider>

ID=(Ar, SIG=3.542, EPS=93.3, frac = 1.0 , deltae = 200.0 , n = 0.0 , tref = 298)

</Collider>

!!=====

<R1>

NAME OH

PARITY Undefined

Symmetry=1

OpticalIsomer=1

EnergyLevel=(-75.65816, 2)

Coordinates

O 0.00000000 0.00000000 0.10835700
H 0.00000000 0.00000000 -0.86685200
Frequency
3704.7381
Scale=0.99
</R1>

<R2>
NAME CHCH
PARITY Undefined
Symmetry=2
!!Symmetry = 1
OpticalIsomer=1
EnergyLevel=(-77.214409,1)
Coordinates
C 0.00000000 0.00000000 0.59902600
H 0.00000000 0.00000000 1.66135000
C 0.00000000 0.00000000 -0.59902600
H 0.00000000 0.00000000 -1.66135000
FREQUENCY
638.9236 638.9236 769.6514
769.6514 2070.5056 3425.8579
3528.5686
Scale=0.99
</R2>

<TS-R-IM1>
NAME C2H2-OH_CHCHOH
Symmetry=1
OpticalIsomer=1
EnergyLevel=(-152.873128, 2) !!original
Tunneling=Eckart
Coordinates
C -0.55207300 0.62580900 0.03157600
H -0.15537300 1.61104000 0.08219200
C -1.25460900 -0.36029900 -0.01881200
H -1.79362400 -1.27475500 -0.08297500
O 1.43306700 -0.13805300 -0.08370400
H 1.32455700 -0.82492500 0.59382600
FREQUENCY
-256.5398 85.5106 246.5271
612.8470 643.0704 672.1907
770.5411 787.1250 1973.3513
3416.2442 3504.4531 3752.6748
Scale=0.99
</TS-R-IM1>

```

<IM1>
Name CHCHOH
Symmetry=1
OpticalIsomer=1
EnergyLevel=(-152.930072,2)
LJPARAMeter=(EPSILON=436.0, SIGMA=3.97)
Coordinates
C      0.11180500  0.38767100 -0.00013500
H      0.10499000  1.47819100  0.00025300
C      1.22734600 -0.30179100 -0.00000200
H      2.28887400 -0.13391800  0.00021300
O     -1.16407800 -0.09947300  0.00004500
H     -1.11614500 -1.06376900 -0.00000200
FREQUENCY
474      480      577
770.9786    845.0895    1106.3025
1249.6166    1364.8478    1672.0399
3099.8113    3300.4924    3790.5949
Scale=0.99

```

```

!*
AnHarm
474 480 577
-5.0
-5.0 -5.0
-5.0 -5.0 -5.0
*!

```

```

</IM1>

```

```

<TS-IM1-P1>
NAME CHCHOH_CH2CHOJ
Symmetry=1
EnergyLevel=(-152.868377, 2) !!original
!!EnergyLevel=(-152.930072,2) !!fake
Tunneling=Eckart
Coordinates
C      -0.00097500  0.53372300 -0.01556000
H      0.14452500  1.61171700 -0.01725900
C     -1.10561100 -0.30881200 -0.03414600
H     -2.11829000  0.03179400  0.18735200
O      1.05143100 -0.23642600  0.02161200
H      0.20182900 -1.10156600 -0.04475200
FREQUENCY
-1961.3341    293.3987    816.1764
 911.8011    1014.0462    1100.0497
1168.7527    1308.1982    1405.4835

```

```

2007.2122      3115.2840      3163.1271
Scale=0.99
</TS-IM1-P1>

<Outlet1>
Name CH2dCHOj
Symmetry=1
OpticalIsomer=1
EnergyLevel=(-152.97512,2)
LJPARAMeter=(EPSILON=436.0, SIGMA=3.97)
Coordinates
C   1.055667000  -0.528211000   0.000000000
H   2.095014000  -0.221283000   0.000000000
H   0.809252000  -1.583503000   0.000000000
C   0.000000000   0.427899000   0.000000000
H   0.297374000   1.494278000   0.000000000
O  -1.191955000   0.114047000   0.000000000
Frequency
451.0390      505.2945      756.6299
975.3570      980.0742     1150.9088
1396.7912     1470.4036     1553.1200
2927.2254     3137.8023     3253.6025
Scale=0.99
</Outlet1>

<Product1>
Name CH2dCHOj
Components 1
</Product1>

```

Text S2: MSMC input for C₂H₅ + O₂ system

```
<Description>
Test case for C2H5+O2
</Description>

<NodeNumber>
2
</NodeNumber>

<CoreNumber>
4
</CoreNumber>

<Precision>
256
</Precision>

<ELMT>
CBS-QB3
</ELMT>

<debug>
on
</debug>

<PESPrint>
on
</PESPrint>

<Temperature>!!Unit: K
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
```

```

1900
2000
</Temperature>

<Pressure>!!Unit: torr
760
</Pressure>

<nasafit>
off
</nasafit>

<arrhfit>
modified
</arrhfit>

<Kinetics>
Profiles = none
Init = C2H5
BoltzmannReactant = On
NM = 1.0E-03 !!Unit: molecule/cm^3
Omega = Lennard-Jones
Deter = (mpack, high)
</Kinetics>

<EnergyStep>!!Unit: cm^-1
200.00
</EnergyStep>

<Collider>
Id = (He , sig = 2.55 , eps = 10.0 , frac = 1.0 , deltae = 190.0 , n = 0.0 , tref = 298)
!! DOI:10.1021/jp0451142
</Collider>

<R1>
NAME C2H5
Symmetry=1
PARITY Undefined
OpticalIsomer=1
EnergyLevel=(-79.030542, 2)
Coordinates
C      0.01005600 -0.69327500  0.00000000
H      -1.01294700 -1.10568200  0.00000000
H       0.50582600 -1.10169900  0.88614200
H       0.50582600 -1.10169900 -0.88614200
C      0.01005600  0.79444000  0.00000000
H      -0.05968600  1.35104400  0.92637000
H      -0.05968600  1.35104400 -0.92637000

```


FREQUENCY

109.3909	477.4249	813.2866
980.0275	1061.9602	1191.6141
1400.8647	1465.0228	1482.6418
1482.9515	2940.8518	3033.6447
3076.9348	3138.6070	3238.2873

Scale=0.99

HinderedRotor=(HinMode=1, HinSym=6, HinAxis=1-5, HinGroup=1,2,3,4)

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

85.69	0.00
95.69	0.02
105.69	0.05
115.69	0.08
125.69	0.08
135.69	0.05
145.69	0.02
155.69	0.00
165.69	0.02
175.69	0.08
-174.31	0.07
-164.31	0.02
-154.31	0.00
-144.31	0.02
-134.31	0.06
-124.31	0.08
-114.31	0.08
-104.31	0.05
-94.31	0.01
-84.31	0.00
-74.31	0.02
-64.31	0.07
-54.31	0.07
-44.31	0.02
-34.31	0.00
-24.31	0.02
-14.31	0.06
-4.31	0.08
5.69	0.08
15.69	0.05
25.69	0.01
35.69	0.00
45.69	0.03
55.69	0.08
65.69	0.07
75.69	0.02
85.69	0.00

</R1>

```

<R2>
NAME O2
Symmetry=2
Parity Odd
Optical_Isomer=1
EnergyLevel=(-150.168252, 3)
Coordinates
O      0.00000000  0.00000000  0.07718700
O      0.00000000  0.00000000  1.28281300
Frequency
1641.2187
Scale=0.99
</R2>

<IM1>
Name C2H5O2
LJPARAMeter=(EPSILON=467.3, SIGMA=4.94)
Symmetry=1
OpticalIsomer=1
EnergyLevel=(-229.261988, 2)
COORDINATES
C      -1.46361700 -0.47537000 -0.09195500
C      -0.49965200  0.64237900  0.25536600
O       0.80007200  0.43255300 -0.38226900
O       1.45468900 -0.56605500  0.17561000
H      -0.31833600  0.71669400  1.32894000
H      -2.42879500 -0.29628500  0.38895700
H      -1.62058400 -0.53411800 -1.17120000
H      -1.07134300 -1.43020700  0.26126200
H      -0.81942000  1.60987900 -0.13514800
FREQUENCY
116.7915      234.5468      358.4345
529.9754      800.5442      844.2614
993.5872     1097.9489     1151.1675
1202.0581     1308.3070     1377.5958
1409.6847     1482.0252     1486.8144
1506.3816     3040.2811     3064.7443
3105.7147     3112.9228     3132.6945
Scale=0.99
HinderedRotor=(HinMode=1, HinSym=1, HinAxis=2-3, HinGroup=3,4)
HindrancePotential
  theta  dE0 [kcal/mol]
  -71.40   0.00
  -61.40   0.13
  -51.40   0.49
  -41.40   0.96

```

-31.40	1.41
-21.40	1.76
-11.40	1.98
-1.40	2.07
8.60	2.02
18.60	1.83
28.60	1.52
38.60	1.09
48.60	0.62
58.60	0.22
68.60	0.02
78.60	0.06
88.60	0.28
98.60	0.55
108.60	0.80
118.60	0.95
128.60	0.98
138.60	0.90
148.60	0.76
158.60	0.58
168.60	0.43
178.60	0.37
-171.40	0.41
-161.40	0.54
-151.40	0.71
-141.40	0.87
-131.40	0.97
-121.40	0.97
-111.40	0.85
-101.40	0.63
-91.40	0.35
-81.40	0.10
-71.40	0.00

HinderedRotor=(HinMode=2, HinSym=3, HinAxis=1-2, HinGroup=1,6,7,8)

HindrancePotential

theta	dE0 [kcal/mol]
-179.66	0.00
-169.66	0.19
-159.66	0.71
-149.66	1.46
-139.66	2.27
-129.66	2.93
-119.66	3.20
-109.66	2.99
-99.66	2.36
-89.66	1.54
-79.66	0.76
-69.66	0.20

-59.66	0.00
-49.66	0.20
-39.66	0.76
-29.66	1.54
-19.66	2.35
-9.66	2.96
0.34	3.20
10.34	3.00
20.34	2.43
30.34	1.62
40.34	0.82
50.34	0.23
60.34	0.00
70.34	0.19
80.34	0.74
90.34	1.53
100.34	2.36
110.34	2.98
120.34	3.20
130.34	2.93
140.34	2.29
150.34	1.47
160.34	0.71
170.34	0.19
-179.66	0.00

</IM1>

<IM2>

Name C2H4OOH

LJPARAMeter=(EPSILON=467.3, SIGMA=4.94)

Symmetry=1

Parity Undefined

OpticalIsomer=1

EnergyLevel=(-229.231563, 2)

COORDINATES

C	-1.49589100	-0.55147500	-0.09786400
C	-0.63007800	0.60444400	0.24732200
O	0.65608600	0.56694300	-0.38709600
O	1.41895500	-0.49818800	0.24039500
H	-2.06100100	-1.08428200	0.65545900
H	-1.59733500	-0.85097200	-1.13469800
H	-0.50012800	0.70962300	1.32876100
H	1.35444600	-1.19079500	-0.43149100
H	-1.04049500	1.54857000	-0.14117000

FREQUENCY

117.3824	162.7957	221.0660
357.3773	469.2429	571.5328
834.2842	861.6758	953.3132

1056.6344	1136.5401	1272.8955
1362.9643	1370.8436	1446.5044
1460.3111	2982.7459	3057.0435
3138.3361	3248.6642	3765.4762

Scale=0.99

HinderedRotor=(HinMode=1, HinSym=2, HinAxis=1-2, HinGroup=1,5,6)

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

135.19	0.00
--------	------

145.19	0.02
--------	------

155.19	0.11
--------	------

165.19	0.29
--------	------

175.19	0.57
--------	------

-174.81	0.92
---------	------

-164.81	0.79
---------	------

-154.81	0.68
---------	------

-144.81	0.62
---------	------

-134.81	0.57
---------	------

-124.81	0.52
---------	------

-114.81	0.46
---------	------

-104.81	0.39
---------	------

-94.81	0.31
--------	------

-84.81	0.23
--------	------

-74.81	0.15
--------	------

-64.81	0.08
--------	------

-54.81	0.02
--------	------

-44.81	0.01
--------	------

-34.81	0.10
--------	------

-24.81	0.32
--------	------

-14.81	0.58
--------	------

-4.81	0.80
-------	------

5.19	0.93
------	------

15.19	0.93
-------	------

25.19	0.84
-------	------

35.19	0.71
-------	------

45.19	0.61
-------	------

55.19	0.52
-------	------

65.19	0.41
-------	------

75.19	0.31
-------	------

85.19	0.23
-------	------

95.19	0.16
-------	------

105.19	0.10
--------	------

115.19	0.05
--------	------

125.19	0.01
--------	------

135.19	0.00
--------	------

HinderedRotor=(HinMode=2, HinSym=1, HinAxis=2-3, HinGroup=3,4,8)

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

-71.08	0.00
-61.08	0.29
-51.08	1.12
-41.08	2.32
-31.08	3.64
-21.08	4.81
-11.08	5.60
-1.08	5.87
8.92	5.40
18.92	4.64
28.92	3.53
38.92	2.34
48.92	1.30
58.92	0.63
68.92	0.49
78.92	0.87
88.92	1.61
98.92	2.45
108.92	2.67
118.92	2.69
128.92	2.36
138.92	1.81
148.92	1.19
158.92	0.69
168.92	0.48
178.92	0.62
-171.08	0.71
-161.08	1.00
-151.08	1.51
-141.08	2.09
-131.08	2.57
-121.08	2.76
-111.08	2.49
-101.08	1.86
-91.08	1.08
-81.08	0.29
-71.08	0.00

HinderedRotor=(HinMode=3, HinSym=1, HinAxis=3-4, HinGroup=4,8)

HindrancePotential

theta dE0 [kcal/mol

102.91	0.00
112.91	0.07
122.91	0.22
132.91	0.40
142.91	0.59
152.91	0.74
162.91	0.85
172.91	0.90

-177.09	0.91
-167.09	0.86
-157.09	0.78
-147.09	0.68
-137.09	0.58
-127.09	0.50
-117.09	0.47
-107.09	0.52
-97.09	0.68
-87.09	0.96
-77.09	1.39
-67.09	1.97
-57.09	2.68
-47.09	3.51
-37.09	4.36
-27.09	5.12
-17.09	5.64
-7.09	5.82
2.91	5.61
12.91	5.05
22.91	4.24
32.91	3.30
42.91	2.37
52.91	1.55
62.91	0.91
72.91	0.46
82.91	0.17
92.91	0.03
102.91	0.00

</IM2>

<TS-R-IM1>

NAME C2H5+O2_C2H5O2

PreExponential 14.831E-13 !! Bimolecular rxn Unit: cm³/molecule/s based on Hans-Heinrich et al.
(DOI:10.1021/jp0451142)

Exponential 0.52

ActivationEnergy 0.0 !! Unit: K

</TS-R-IM1>

<TS-IM1-IM2>

NAME C2H5O2_C2H4OOH

EnergyLevel=(-229.19831, 2)

Symmetry=1

Parity Undefined

OpticalIsomer=1

Tunneling=Eckart

Coordinates

C 1.22499600 -0.56702800 -0.11990500

C	0.54021700	0.75440400	0.21265600
O	-0.79240300	0.59629900	-0.29197000
O	-1.14078400	-0.70011300	0.16211700
H	-0.02955300	-1.13787400	0.06146000
H	0.95909100	1.62852600	-0.29316000
H	1.94864400	-0.96652400	0.58533400
H	1.47124800	-0.73395000	-1.16696100
H	0.52479100	0.91607400	1.29564500

FREQUENCY

-2273.9888	275.5101	439.9312
553.9176	690.6842	869.2051
897.8081	903.1570	959.7678
1043.9316	1112.4091	1166.1895
1245.6413	1343.9535	1454.1942
1497.3342	1728.0249	3025.7684
3084.1658	3099.2958	3192.1739

Scale=0.99

</TS-IM1-IM2>

<TS-IM1-P1>

NAME C2H5O2_C2H4-HO2(C)

Scale=0.99

EnergyLevel=(-229.205705, 2)

Symmetry=1

Parity Undefined

OpticalIsomer=1

Tunneling=Eckart

Coordinates

C	1.05019800	0.74547400	0.00011800
C	1.28440000	-0.61979500	0.00003200
O	-1.14915900	0.61613700	-0.00011200
O	-1.26234100	-0.64853400	0.00004800
H	-0.03219300	-0.95505000	-0.00104900
H	1.02800200	1.31968300	0.91734900
H	1.02917000	1.31983500	-0.91705600
H	1.63047900	-1.08944000	-0.91739600
H	1.62895300	-1.08993000	0.91776600

FREQUENCY

-1099.1262	218.6724	359.1594
480.1130	517.8001	643.2699
834.1963	889.1725	1005.3797
1040.9016	1228.5187	1303.5575
1315.3738	1341.4865	1470.1616
1570.7688	1604.7107	3099.6101
3158.0062	3177.1480	3246.1353

</TS-IM1-P1>

<TS-IM1-P2>

NAME C2H5O2_CCHO-OH

EnergyLevel=(-229.189419, 2)

Symmetry=1

Parity Undefined

OpticalIsomer=2 !! double-check

Tunneling=Eckart

Coordinates

C	1.61750900	-0.17237600	-0.22417300
C	0.33216000	0.05523100	0.51251400
O	-0.65529000	0.73867900	-0.18644100
O	-1.51985900	-0.48626900	-0.12969400
H	2.13318600	0.78352000	-0.37730200
H	-0.50326200	-0.98039400	0.46922600
H	2.28152200	-0.83092000	0.34027000
H	1.42259100	-0.60726800	-1.20639200
H	0.36914000	0.31865500	1.57323200

FREQUENCY

-1842.4558	133.3782	206.2576
416.8852	656.5526	780.5559
797.0365	912.3736	1057.9303
1113.5882	1118.1073	1162.4026
1355.4106	1407.9920	1473.7655
1479.3115	1947.0655	3013.8935
3064.8889	3082.4506	3119.0744

HinderedRotor=(HinMode=2, HinSym=3, HinAxis=1-2, HinGroup=1,5,7,8) !!exclude the imaginary

HindrancePotential

theta dE0 [kcal/mol]

68.28	0.00
78.28	0.15
88.28	0.55
98.28	1.12
108.28	1.72
118.28	2.15
128.28	2.30
138.28	2.11
148.28	1.65
158.28	1.05
168.28	0.50
178.28	0.12
-171.72	0.00
-161.72	0.17
-151.72	0.59
-141.72	1.16
-131.72	1.74
-121.72	2.16
-111.72	2.30

```

-101.72  2.13
-91.72   1.70
-81.72   1.13
-71.72   0.58
-61.72   0.17
-51.72   0.00
-41.72   0.13
-31.72   0.53
-21.72   1.11
-11.72   1.71
-1.72    2.16
 8.28    2.30
18.28    2.09
28.28    1.63
38.28    1.05
48.28    0.51
58.28    0.13
68.28    0.00
Scale = 0.99
</TS-IM1-P2>

<TS-IM2-P3>
NAME C2H4OOH_C2H4-HO2(b-s)
Scale=0.99
EnergyLevel=(-229.205154, 2)
Symmetry=1
Parity Undefined
OpticalIsomer=1
Tunneling=Eckart
Coordinates
C      1.62284900  0.53686500 -0.11542200
C      0.92189400 -0.55108600  0.36259500
O     -0.76081200 -0.47094400 -0.48530400
O     -1.61106600  0.34853900  0.25457100
H      1.54724500  1.50651500  0.36274900
H      2.18043200  0.48198600 -1.04248300
H      0.51666500 -0.53199400  1.36664400
H     -1.67236400  1.14565900 -0.29173600
H      1.13458700 -1.53760500 -0.03235200
FREQUENCY
-537.2979      96.5583      229.6776
 313.0231      422.0756      474.5590
 816.8560      822.2708      918.1757
1031.6991     1083.2572     1239.0800
1259.2651     1382.9124     1464.6052
1545.1332     3137.3725     3142.1358
3215.7015     3241.0711     3728.0034
HinderedRotor=(HinMode=1, HinSym=1, HinAxis=2-3, HinGroup=3,4,8) !!exclude the imaginary

```

HindrancePotential

theta dE0 [kcal/mol]

-86.40	0.00
-76.40	0.09
-66.40	0.36
-56.40	0.79
-46.40	1.33
-36.40	1.94
-26.40	2.52
-16.40	2.99
-6.40	3.30
3.60	3.40
13.60	3.29
23.60	3.00
33.60	2.60
43.60	2.14
53.60	1.71
63.60	1.36
73.60	1.13
83.60	1.07
93.60	1.13
103.60	1.27
113.60	1.46
123.60	1.63
133.60	1.77
143.60	1.86
153.60	1.90
163.60	1.91
173.60	1.89
-176.40	1.87
-166.40	1.82
-156.40	1.70
-146.40	1.51
-136.40	1.25
-126.40	0.93
-116.40	0.60
-106.40	0.30
-96.40	0.09
-86.40	0.01

HinderedRotor=(HinMode=4, HinSym=1, HinAxis=3-4, HinGroup=4,8) !!exclude the imaginary

HindrancePotential

theta dE0 [kcal/mol]

107.15	0.00
117.15	0.20
127.15	0.75
137.15	1.59
147.15	2.69
157.15	4.01

167.15	5.50
177.15	7.09
-172.85	8.65
-162.85	9.89
-152.85	8.45
-142.85	6.86
-132.85	5.34
-122.85	3.94
-112.85	2.74
-102.85	1.83
-92.85	1.26
-82.85	1.06
-72.85	1.25
-62.85	1.81
-52.85	2.72
-42.85	3.91
-32.85	5.32
-22.85	6.85
-12.85	8.44
-2.85	9.97
7.15	11.34
17.15	12.23
27.15	8.37
37.15	6.85
47.15	5.32
57.15	3.86
67.15	2.54
77.15	1.45
87.15	0.64
97.15	0.16
107.15	0.01
</TS-IM2-P3>	
<TS-IM2-P4>	
NAME CjCOOH_cyCCO+OH	
Scale=0.99	
EnergyLevel=(-229.2078027, 2)	
Symmetry=1	
Parity Undefined	
OpticalIsomer=1	
Tunneling=Eckart	
Coordinates	
C	-1.70198500 -0.25736600 0.05651100
C	-0.58464500 0.70368400 0.02174000
O	0.20020600 -0.44259900 -0.14198700
O	1.88106800 0.04584400 -0.00353600
H	-1.97713300 -0.73166600 0.98786000

H	-2.14311400	-0.61683300	-0.86244300
H	-0.39191800	1.23251200	0.95882500
H	2.13978000	-0.77273800	0.44376100
H	-0.55802400	1.38485500	-0.83331900

FREQUENCY

-737.4492	85.0359	123.0790
257.1079	390.9873	495.9172
763.2849	836.4830	937.3066
1002.5935	1166.1663	1168.5617
1200.6425	1313.8595	1467.7256
1535.6212	3029.5544	3083.5689
3164.9885	3281.0621	3788.8377

HinderedRotor=(HinMode=2, HinSym=1, HinAxis=3-4, HinGroup=4,8) !!exclude the imaginary

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

144.12	0.00
154.12	0.03
164.12	0.07
174.12	0.10
175.88	0.10
165.88	0.07
155.88	0.03
145.88	0.00
135.88	0.00
125.88	0.03
115.88	0.12
105.88	0.30
-95.88	0.57
-85.88	0.94
-75.88	1.40
-65.88	1.96
-55.88	2.58
-45.88	3.24
-35.88	3.89
-25.88	4.47
-15.88	4.95
-5.88	5.26
4.12	5.30
14.12	5.02
24.12	4.57
34.12	4.00
44.12	3.36
54.12	2.70
64.12	2.07
74.12	1.50
84.12	1.02
94.12	0.63
104.12	0.35

114.12	0.15
124.12	0.04
134.12	0.00
144.12	0.00

</TS-IM2-P4>

<Outlet1>

Name C2H4

Scale=0.99

Symmetry=4

PARITY Undefined

OpticalIsomer=1

EnergyLevel=(-78.467449, 1)

Coordinate

C	0.00000000	0.66347200	0.00000000
C	0.00000000	-0.66347200	0.00000000
H	0.92251800	1.23459900	0.00000100
H	-0.92251800	1.23459900	0.00000100
H	-0.92251800	-1.23459900	0.00000100
H	0.92251800	-1.23459900	0.00000100

Frequency

834.4967	972.7314	973.4198
1066.3907	1238.5732	1379.5821
1472.1287	1691.8441	3121.8038
3136.9408	3193.0573	3221.5077

</Outlet1>

<Outlet2>

Name HO2

Scale=0.99

Symmetry=1

PARITY Undefined

OpticalIsomer=1

EnergyLevel=(-150.755227, 2)

Coordinate

O	0.05528900	-0.60941600	0.00000000
H	-0.88463000	-0.87113300	0.00000000
O	0.05528900	0.71830800	0.00000000

Frequency

1164.9194	1428.5061	3606.9913
-----------	-----------	-----------

</Outlet2>

<Outlet3>

Name CH3CHO

Scale=0.99

Symmetry=1

PARITY Undefined

OpticalIsomer=1

EnergyLevel=(-153.637676, 1)

Coordinate

C	1.16883600	-0.14777800	-0.00000900
C	-0.23561000	0.39720300	-0.00001100
O	-1.23314400	-0.27657000	0.00000100
H	1.70780600	0.22253400	-0.87890900
H	1.70768600	0.22227100	0.87909300
H	-0.30511100	1.50870400	0.00004300
H	1.15541500	-1.23749300	-0.00011800

Frequency

160.1833	508.1924	776.7180
882.5968	1125.5861	1135.2928
1374.6562	1425.8709	1460.3871
1470.9204	1824.0273	2856.2355
3021.5533	3076.6246	3136.3551

HinderedRotor=(HinMode=1, HinSym=3, HinAxis=1-2, HinGroup=1,4,5,7) !!exclude the imaginary

HindrancePotential

theta	dE0 [kcal/mol]
121.58	0.00
131.58	0.06
141.58	0.22
151.58	0.46
161.58	0.73
171.58	0.93
-178.42	0.98
-168.42	0.87
-158.42	0.65
-148.42	0.38
-138.42	0.16
-128.42	0.03
-118.42	0.00
-108.42	0.09
-98.42	0.26
-88.42	0.50
-78.42	0.74
-68.42	0.92
-58.42	0.99
-48.42	0.91
-38.42	0.71
-28.42	0.46
-18.42	0.21
-8.42	0.05
1.58	0.00
11.58	0.09
21.58	0.28
31.58	0.54
41.58	0.79
51.58	0.95

61.58 0.98
71.58 0.87
81.58 0.66
91.58 0.42
101.58 0.20
111.58 0.05
121.58 0.00

</Outlet3>

<Outlet4>

Name OH

Scale=0.99

Symmetry=1

PARITY Undefined

OpticalIsomer=1

EnergyLevel=(-75.658133, 2)

Coordinate

O	0.00000000	0.00000000	0.10835700
H	0.00000000	0.00000000	-0.86685500

Frequency

3704.6968

</Outlet4>

<Outlet5>

Name cyCCO

Scale=0.99

Symmetry=2

PARITY Undefined

OpticalIsomer=1

EnergyLevel=(-153.5963876, 1)

Coordinate

C	0.00000000	0.73384200	-0.37184700
H	0.91912800	1.27008000	-0.59441400
H	-0.92025800	1.26869100	-0.59386500
C	0.00000000	-0.73384200	-0.37184700
H	0.92025800	-1.26869100	-0.59386500
O	0.00000000	0.00000000	0.85484100
H	-0.91912800	-1.27008000	-0.59441400

Frequency

818.3726	843.3580	889.6657
1039.1049	1139.1615	1141.9109
1167.6774	1171.8659	1300.3290
1504.0082	1540.2137	3077.2326
3084.8781	3158.2361	3173.6983

</Outlet5>

<Product1>

Name C2H4+HO2_c

Components 1 2

</Product1>

<Product2>

Name CH3CHO+OH

Components 3 4

</Product2>

<Product3>

Name C2H4+HO2_beta-s

Components 1 2

</Product3>

<Product4>

Name cyCCO+OH

Components 4 5

</Product4>

Text S3: MSMC input for CH₃OC(=O) decomposition

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Test case for decomposition of CH3OC(=O) and CH2OC(=O)H
Ref: 10.1021/acs.jpcc.5b07959
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800
900
1000
1100
1200
1300
1400
1500
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1800
1900
2000
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</Pressure>

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on
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Profiles=none
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Omega = Lennard-Jones
Deter = (mpack, high) !! (Diagonalize method , Grid resolution)
Stoch = (msmc, boost, 1.0E+07)
</Kinetics>

<EnergyStep>!!Unit: cm^-1
200.0
</EnergyStep>

<Collider>
ID=(N2, SIG=3.74, EPS=82.0, FRAC=1.0, DELTAE=250.0, N=0.8, TREF=298)
!! Tan et al. (JPCB 2016)
</Collider>

<IM1>
Name i1
Symmetry=1
PARITY Undefined
OpticalIsomer=1
LJPARAMeter=(EPSILON=406.457, SIGMA=4.71) !! based on Tan et al.
EnergyLevel = (-228.130483, 2) !! hartree
Coordinates !! Angstrom
C -0.823692 0.509172 0.000004
O -1.430153 -0.512106 -0.000002
O 0.471427 0.736598 -0.000001

```

C 1.331900 -0.449953 0.000000
H 1.135967 -1.042451 -0.893574
H 1.136370 -1.042147 0.893864
H 2.348221 -0.066653 -0.000290

FREQUENCY !! cm⁻¹

93.4897	272.7022	383.9352
761.8625	877.8623	1133.4537
1147.1904	1188.5681	1453.4000
1482.2922	1488.9481	1847.1792
3057.9062	3140.4733	3177.1275

Scale = 0.990

HinderedRotor = (HinFreq = 383.9352, HinSym = 1, HinAxis = 1 - 3, HinGroup = 1, 2)

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

-0.1	0.0000
------	--------

9.9	0.2698
-----	--------

19.9	1.0668
------	--------

29.9	2.2841
------	--------

39.9	3.7713
------	--------

49.9	5.3715
------	--------

59.9	6.9089
------	--------

69.9	8.1702
------	--------

79.9	8.9859
------	--------

89.9	9.2369
------	--------

99.9	8.8981
------	--------

109.9	8.0321
-------	--------

119.9	6.7583
-------	--------

129.9	5.2585
-------	--------

139.9	3.7149
-------	--------

149.9	2.3155
-------	--------

159.9	1.2174
-------	--------

169.9	0.5459
-------	--------

179.9	0.3389
-------	--------

-170.1	0.5334
--------	--------

-160.1	1.1923
--------	--------

-150.1	2.2841
--------	--------

-140.1	3.6772
--------	--------

-130.1	5.2146
--------	--------

-120.1	6.7206
--------	--------

-110.1	8.0007
--------	--------

-100.1	8.8793
--------	--------

-90.1	9.2369
-------	--------

-80.1	8.9985
-------	--------

-70.1	8.2015
-------	--------

-60.1	6.9465
-------	--------

-50.1	5.4154
-------	--------

-40.1	3.8153
-------	--------

-30.1	2.3218
-------	--------

-20.1	1.0981
-10.1	0.2887
-0.1	0.0000

HinderedRotor = (HinFreq = 93.4897, HinSym = 3, HinAxis = 3 - 4, HinGroup = 1, 2, 3)

HindrancePotential

theta	dE0 [kcal/mol]
59.5	0.0000
69.5	0.0377
79.5	0.1443
89.5	0.2887
99.5	0.4330
109.5	0.5334
119.5	0.5773
129.5	0.5522
139.5	0.4644
149.5	0.3263
159.5	0.1757
169.5	0.0565
179.5	0.0063
-170.5	0.0439
-160.5	0.1569
-150.5	0.3075
-140.5	0.4518
-130.5	0.5522
-120.5	0.5836
-110.5	0.5459
-100.5	0.4455
-90.5	0.3075
-80.5	0.1569
-70.5	0.0439
-60.5	0.0000
-50.5	0.0439
-40.5	0.1569
-30.5	0.3012
-20.5	0.4455
-10.5	0.5459
-0.5	0.5836
9.5	0.5522
19.5	0.4581
29.5	0.3200
39.5	0.1694
49.5	0.0502
59.5	0.0000

</IM1>

<IM2>

Name i2

Symmetry=1

```

PARITY Undefined
OpticalIsomer=1
LJPARAMeter=(EPSILON=406.457, SIGMA=4.71) !! based on Tan et al.
EnergyLevel = (-228.128004, 2) !! hartree
Coordinates !! Angstrom
C  0.771716  0.446762  0.000051
O  1.314175 -0.619085 -0.000015
O  -0.577583  0.645612 -0.000020
C  -1.396910 -0.447049 -0.000026
H  -0.956243 -1.430507  0.000061
H  -2.446113 -0.207771  0.000111
H  1.260788  1.427791 -0.000048
FREQUENCY !! cm^-1
  139.2528      263.5127      326.9505
  380.4800      751.1723      997.1314
 1005.5978     1158.3997     1220.4681
 1399.3324     1443.4705     1807.6786
 3067.1437     3181.2273     3342.3733
Scale = 0.990
!*
HinderedRotor = (HinFreq = 380.48, HinSym = 1, HinAxis = 1 - 3, HinGroup = 1, 2, 7)
HindrancePotential
  theta      dE0 [kcal/mol]
  -0.0        0.0000
   10.0        0.2698
   20.0        1.1609
   30.0        2.5979
   40.0        4.4428
   50.0        6.5135
   60.0        8.5843
   70.0       10.3916
   80.0       11.6780
   90.0       12.2615
  100.0       12.0796
  110.0       11.2763
  120.0       10.0527
  130.0        8.6471
  140.0        7.2352
  150.0        5.9864
  160.0        5.0075
  170.0        4.3737
  180.0        4.1039
 -170.0        4.2357
 -160.0        4.7753
 -150.0        5.6915
 -140.0        6.9403
 -130.0        8.4212
 -120.0        9.9774

```

-110.0	11.4207
-100.0	12.4937
-90.0	12.9581
-80.0	12.6380
-70.0	11.5148
-60.0	8.5969
-50.0	6.5261
-40.0	4.4553
-30.0	2.6042
-20.0	1.1672
-10.0	0.2761
-0.0	0.0000

*!

HinderedRotor = (HinFreq = 263.5127, HinSym = 2, HinAxis = 3 - 4, HinGroup = 4, 5, 6)

HindrancePotential

theta	dE0 [kcal/mol]
-0.0	0.0000
10.0	-0.0188
20.0	0.1255
30.0	0.4895
40.0	1.0793
50.0	1.8763
60.0	2.8050
70.0	3.7964
80.0	4.7063
90.0	5.3966
100.0	4.7377
110.0	3.9596
120.0	3.0622
130.0	2.1398
140.0	1.2989
150.0	0.6275
160.0	0.1820
170.0	-0.0126
180.0	0.0000
-170.0	-0.0126
-160.0	0.1757
-150.0	0.6212
-140.0	1.2989
-130.0	2.1335
-120.0	3.0560
-110.0	3.9533
-100.0	4.7314
-90.0	5.2648
-80.0	5.4468
-70.0	3.7964
-60.0	2.8112
-50.0	1.8763

```

-40.0      1.0856
-30.0      0.4895
-20.0      0.1255
-10.0     -0.0188
-0.0       0.0000
</IM2>

<TS-IM1-P2>
Name ts1
Symmetry=1
PARITY Undefined
OpticalIsomer=1
Tunneling = Eckart
EnergyLevel = (-228.090974, 2) !! hartree
Coordinates !! Angstrom
C  -1.037731  0.471117  0.000016
O  -2.016271 -0.100271 -0.000010
O   0.646355 -0.565748  0.000006
C   1.794937  0.221514 -0.000005
H   1.895931  0.837809  0.901352
H   1.895726  0.838100 -0.901186
H   2.624431 -0.503543 -0.000202
FREQUENCY !! cm^-1
-298.0234      93.9672      157.6755
 200.7393      326.3107      995.7688
1121.1204      1145.2206      1412.4320
1415.1888      1511.5168      2148.6058
2962.2553      3019.5164      3049.8548
Scale = 0.990
HinderedRotor = (HinFreq = 93.9672, HinSym = 1, HinAxis = 1 - 3, HinGroup = 1, 2)
HindrancePotential
  theta      dE0 [kcal/mol]
 179.7      0.0000
-170.3      0.0439
-160.3      0.1757
-150.3      0.3828
-140.3      0.6589
-130.3      0.9915
-120.3      1.3554
-110.3      1.7194
-100.3      2.0708
-90.3       2.3908
-80.3       2.6732
-70.3       2.9116
-60.3       3.1250
-50.3       3.3133
-40.3       3.4764
-30.3       3.6207

```


-20.3	3.7274
-10.3	3.8027
-0.3	3.8278
9.7	3.8027
19.7	3.7337
29.7	3.6270
39.7	3.4890
49.7	3.3258
59.7	3.1438
69.7	2.9367
79.7	2.6920
89.7	2.4159
99.7	2.0959
109.7	1.7445
119.7	1.3805
129.7	1.0166
139.7	0.6840
149.7	0.4016
159.7	0.1883
169.7	0.0502
179.7	0.0063

HinderedRotor = (HinFreq = 157.6755, HinSym = 3, HinAxis = 3 - 4, HinGroup = 4, 5, 6, 7)

HindrancePotential

theta	dE0 [kcal/mol]
64.2	0.0000
74.2	0.0879
84.2	0.3200
94.2	0.6463
104.2	0.9538
114.2	1.1107
124.2	1.1044
134.2	0.9475
144.2	0.6903
154.2	0.4016
164.2	0.1632
174.2	0.0188
-175.8	0.0063
-165.8	0.1255
-155.8	0.3577
-145.8	0.6463
-135.8	0.9162
-125.8	1.0919
-115.8	1.1295
-105.8	0.9977
-95.8	0.7028
-85.8	0.3702
-75.8	0.1192
-65.8	0.0000

```

-55.8      0.0377
-45.8      0.2134
-35.8      0.4769
-25.8      0.7593
-15.8      0.9915
-5.8       1.1170
4.2        1.1232
14.2       1.0166
24.2       0.8032
34.2       0.5208
44.2       0.2447
54.2       0.0565
64.2       0.0000
</TS-IM1-P2>

<TS-IM1-P1>
Name ts2
Symmetry=1
PARITY Undefined
OpticalIsomer=1
Tunneling = Eckart
EnergyLevel = (-228.104312, 2) !! hartree
Coordinates !! Angstrom
C  -0.856961  -0.393365  0.000023
O  -1.578391  0.541521  -0.000007
O   0.302256  -0.799311  -0.000008
C   1.652357  0.445614  -0.000003
H   1.115961  1.386372  -0.003281
H   2.162192  0.179045  -0.915574
H   2.158547  0.183404  0.918852
FREQUENCY !! cm^-1
-730.5802      41.4904      190.5556
504.8731      671.1671      777.8494
790.7517     1065.3057     1177.5510
1433.7477     1438.4310     2034.4256
3103.7151     3257.7212     3266.4635
Scale = 0.990
HinderedRotor = (HinFreq = 41.4904, HinSym = 3, HinAxis = 3 - 4, HinGroup = 4, 5, 6, 7)
HindrancePotential
theta      dE0 [kcal/mol]
-0.4      0.0000
9.6       0.0063
19.6      0.0251
29.6      0.0565
39.6      0.0816
49.6      0.1067
59.6      0.1130

```

69.6	0.1067
79.6	0.0879
89.6	0.0565
99.6	0.0314
109.6	0.0063
119.6	0.0000
129.6	0.0063
139.6	0.0251
149.6	0.0565
159.6	0.0879
169.6	0.1067
179.6	0.1130
-170.4	0.1067
-160.4	0.0879
-150.4	0.0628
-140.4	0.0314
-130.4	0.0063
-120.4	0.0000
-110.4	0.0063
-100.4	0.0251
-90.4	0.0565
-80.4	0.0879
-70.4	0.1067
-60.4	0.1130
-50.4	0.1067
-40.4	0.0879
-30.4	0.0565
-20.4	0.0314
-10.4	0.0063
-0.4	0.0000
</TS-IM1-P1>	
<TS-IM2-P3>	
Name ts3	
Symmetry 2 !! increasing by 2	
Parity = Undefined	
OpticalIsomer = 1	
Tunneling = Eckart	
EnergyLevel = (-228.074755, 2) !! hartree	
Coordinates !! Angstrom	
C	1.024835 0.496439 -0.131984
O	1.427869 -0.608124 0.012022
O	-0.844890 0.631577 0.020405
C	-1.442123 -0.451879 0.017864
H	-0.908884 -1.381509 0.251722
H	-2.499376 -0.491202 -0.261205
H	1.248156 1.417731 0.434785
FREQUENCY !! cm ⁻¹	

-604.6372	178.8111	252.6589
354.9850	496.2496	797.7298
1017.8855	1080.8542	1235.9097
1431.0046	1579.8026	1820.2457
2903.4273	3000.3154	3106.2933

Scale = 0.990

HinderedRotor = (HinFreq = 178.8111, HinSym = 3, HinAxis = 1 - 3, HinGroup = 1, 2, 7)

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

-11.7	0.0000
-------	--------

-1.7	0.3138
------	--------

8.3	1.1923
-----	--------

18.3	2.5477
------	--------

28.3	4.1227
------	--------

38.3	5.5974
------	--------

48.3	6.7583
------	--------

58.3	7.5615
------	--------

68.3	7.9443
------	--------

78.3	6.8148
------	--------

88.3	5.8609
------	--------

98.3	5.1205
------	--------

108.3	4.5557
-------	--------

118.3	4.1290
-------	--------

128.3	3.8466
-------	--------

138.3	3.7211
-------	--------

148.3	3.7400
-------	--------

158.3	3.8906
-------	--------

168.3	4.1667
-------	--------

178.3	4.5243
-------	--------

-171.7	4.9322
--------	--------

-161.7	5.3715
--------	--------

-151.7	5.8170
--------	--------

-141.7	6.2437
--------	--------

-131.7	6.6140
--------	--------

-121.7	6.8838
--------	--------

-111.7	6.9842
--------	--------

-101.7	6.8524
--------	--------

-91.7	6.4633
-------	--------

-81.7	5.8233
-------	--------

-71.7	4.9887
-------	--------

-61.7	4.0412
-------	--------

-51.7	3.0183
-------	--------

-41.7	1.9641
-------	--------

-31.7	0.9664
-------	--------

-21.7	0.2510
-------	--------

-11.7	0.0000
-------	--------

</TS-IM2-P3>

```

<TS-IM1-IM2>
Name ts4
Symmetry 1
Parity = Undefined
OpticalIsomer = 1
Tunneling = Eckart
EnergyLevel = (-228.061753, 2) !! hartree
Coordinates !! Angstrom
C  -0.559904  -0.219178  -0.000009
O  -1.732393  -0.081686   0.000002
O   0.433188   0.676113   0.000008
C   1.527758  -0.279926  -0.000003
H   0.407788  -1.209219  -0.000053
H   2.089320  -0.275845   0.929011
H   2.089406  -0.275722  -0.928966
FREQUENCY !! cm^-1
-2042.4870      214.4563      482.2659
  499.2381      720.6932      903.1651
 1006.2094      1129.4208     1170.7255
 1172.3719      1465.4244     1884.7169
 1927.6333      3099.5921     3221.0681
Scale = 0.990
</TS-IM1-IM2>

```

```

<Outlet1>
NAME ch3
Symmetry=6
PARITY Undefined
OpticalIsomer=1
EnergyLevel = (-39.774075, 2) !! hartree
Coordinates !! Angstrom
C  0.000000  0.000000  0.000044
H  0.000000  1.080512  -0.000087
H  -0.935751  -0.540256  -0.000087
H   0.935751  -0.540256  -0.000087
FREQUENCY !! cm^-1
  505.8187      1403.2795      1403.2812
 3103.6731      3282.7410      3282.7424
Scale = 0.990
</Outlet1>

```

```

<Outlet2>
NAME CO2
Symmetry=2
PARITY Undefined
OpticalIsomer = 1
EnergyLevel = (-188.383698, 1) !! hartree
Coordinates !! Angstrom

```

```

C  0.000000  0.000000  0.000000
O  0.000000  0.000000 -1.160420
O  0.000000  0.000000  1.160420
FREQUENCY !! cm^-1
  666.5589      666.5589      1375.5143
  2435.8827
Scale = 0.990
</Outlet2>

<OUTLET3>
NAME ch3o
Phase = Gas
Symmetry 3
Parity = Undefined
OpticalIsomer = 1
EnergyLevel = (-114.910294, 2) !! hartree
Coordinates !! Angstrom
O -0.791995  0.000000 -0.007689
C  0.573630  0.000002 -0.013980
H  0.871383 -0.000061  1.054523
H  1.011399  0.909266 -0.454519
H  1.011397 -0.909218 -0.454614
FREQUENCY !! cm^-1
  714.5934      963.1040      1107.0138
  1360.4047      1370.8349      1517.5639
  2891.8465      2955.9713      2996.4820
Scale = 0.990
</OUTLET3>

<OUTLET4>
NAME co
Phase = Gas
Symmetry 1
Parity = Undefined
OpticalIsomer = 1
EnergyLevel = (-113.187015, 1) !! hartree
Coordinates !! Angstrom
C  0.000000  0.000000 -0.643977
O  0.000000  0.000000  0.482982
FREQUENCY !! cm^-1
  2219.8190
Scale = 0.990
</OUTLET4>

<OUTLET5>
NAME ch2o
Phase = Gas
Symmetry 2

```

```

Parity = Undefined
OpticalIsomer = 1
EnergyLevel = (-114.370399, 1) !! hartree
Coordinates !! Angstrom
O  -0.674047  -0.000001  0.000000
C  0.525980  0.000000  -0.000001
H  1.118245  0.938676  0.000001
H  1.118254  -0.938671  0.000001
FREQUENCY !! cm^-1
  1202.0872      1270.1376      1538.9918
  1826.5298      2869.7710      2919.1693
Scale = 0.990
</OUTLET5>

<OUTLET6>
NAME hco
Phase = Gas
Symmetry 1
Parity = Undefined
OpticalIsomer = 1
EnergyLevel = (-113.717556, 2) !! hartree
Coordinates !! Angstrom
C  0.062244  0.584087  0.000000
O  0.062244  -0.589992  0.000000
H  -0.871411  1.215409  0.000000
FREQUENCY !! cm^-1
  1110.4127      1942.5290      2624.5144
Scale = 0.990
</OUTLET6>

<Product1>
Name ch3+co2
Components 1 2
</Product1>

<Product2>
Name ch3o+co
Components 3 4
</Product2>

<Product3>
Name ch2o+hco
Components 5 6
</Product3>

```

Text S4: MSMC input for (CH₃CO)₂O decomposition

```
<Description>
This is the MSMC input for the decomposition of acetic anhydride
+ PES @ CCSD(T)/CBS//B3LYP/CBSB7
+ HIR @ B3LYP/6-31G(d)
</Description>

<CoreNumber>
8
</CoreNumber>

<ELMT>
CCSDT-B3LYP
</ELMT>

<debug>
on
</debug>

<PESPrint>
ON
</PESPrint>

<Temperature>!!Unit: K
470
475
500
525
550
575
600
625
643
</Temperature>
<Pressure>!!Unit: torr
7.0
</Pressure>

<ArrheniusFitting>
modified
</ArrheniusFitting>

<NASAfit>
OFF
</NASAfit>
```



```

<Kinetics>
Init = tt-AceticAnhydride
Profiles=None
!!NM = 0.0134
Omega = Lennard-Jones
Deter = (mpack,high) !! (Diagonalize method , Grid resolution)
Stoch = (MSMC,boost,1.0E+07)
</Kinetics>

<EnergyStep>!!Unit: cm^-1
200.0
</EnergyStep>

!*
<TRANSferEnergy>
500.0
</TRANSferEnergy>
*!

<Collider>
ID=(Ar, SIG=3.542, EPS=93.3, FRAC=1.0, DELTAE=500.0, N=0.0, TREF=298)
</Collider>

!*
<Collider>
Name = Ar
Epsilon=93.3
Sigma=3.542
</Collider>
*!

<IM1>
Name tt-AceticAnhydride !! AH[sp,sp]
Symmetry=2
Parity Undefined
OpticalIsomer=1
LJPARAMeter=(EPSILON=454.0, SIGMA=5.413) !! estimated on C4H7O3
(https://combustion.llnl.gov/content/assets/docs/combustion/dme\_24\_tran\_dat.txt)
EnergyLevel = (-381.354311, 1) !! hartree
Coordinates !! Angstrom
C 0.000000 1.217932 -0.090568
O 0.000000 0.000000 0.595723
C 0.000000 -1.217932 -0.090568
C -0.629274 -2.280572 0.766612
H -0.191663 -2.269146 1.766580
H -1.696789 -2.070361 0.873850
H -0.490166 -3.253549 0.300158

```

C	0.629274	2.280572	0.766612
H	0.191663	2.269146	1.766580
H	1.696789	2.070361	0.873850
H	0.490166	3.253549	0.300158
O	0.477485	-1.357154	-1.172468
O	-0.477485	1.357154	-1.172468

FREQUENCY !! cm⁻¹

53.1410	80.0548	118.3411
121.4774	184.4121	334.1549
417.4021	534.5460	557.6539
593.1335	674.1878	806.3364
901.5890	995.1587	1023.3832
1061.0120	1071.5645	1145.8228
1226.1866	1395.8027	1399.3244
1469.5098	1469.5442	1474.3730
1475.6529	1833.7473	1904.0741
3048.9546	3049.1102	3111.3711
3111.3978	3157.6771	3157.8120

Scale = 0.990

HinderedRotor = (HinMode = 1, HinSym = 1, HinAxis = 1 - 2, HinGroup = 1, 8, 9, 10, 11, 13)

HindrancePotential

theta	dE0 [kcal/mol]
-153.6	0.0000
-143.6	0.0941
-133.6	0.3326
-123.6	0.6150
-113.6	0.8409
-103.6	0.9224
-93.6	0.8409
-83.6	0.6714
-73.6	0.4895
-63.6	0.3514
-53.6	0.2510
-43.6	0.2008
-33.6	0.1945
-23.6	0.2510
-13.6	0.3389
-3.6	0.4142
6.4	0.4079
16.4	0.3200
26.4	0.2322
36.4	0.1945
46.4	0.2134
56.4	0.2824
66.4	0.3891
76.4	0.5334
86.4	0.7154

96.4	0.8722
106.4	0.9099
116.4	0.7907
126.4	0.5397
136.4	0.2636
146.4	0.0565
156.4	0.0126
166.4	0.1757
176.4	0.5773
-173.6	0.4455
-163.6	0.1130
-153.6	0.0063

Hindered Rotor = (HinMode = 3, HinSym = 3, HinAxis = 1 - 8, HinGroup = 8, 9, 10, 11)

HindrancePotential

theta	dE0 [kcal/mol]
-171.2	0.0000
-161.2	0.0879
-151.2	0.2510
-141.2	0.4518
-131.2	0.6212
-121.2	0.7216
-111.2	0.7279
-101.2	0.6589
-91.2	0.5146
-81.2	0.3451
-71.2	0.1820
-61.2	0.0565
-51.2	0.0126
-41.2	0.0628
-31.2	0.2008
-21.2	0.3953
-11.2	0.5836
-1.2	0.7091
8.8	0.7342
18.8	0.6589
28.8	0.5020
38.8	0.3200
48.8	0.1443
58.8	0.0314
68.8	0.0063
78.8	0.0753
88.8	0.2196
98.8	0.4016
108.8	0.5773
118.8	0.6965
128.8	0.7342
138.8	0.6903
148.8	0.5522

158.8	0.3765
168.8	0.1883
178.8	0.0502
-171.2	0.0188

!*

Hindered Rotor = (HinMode = 2, HinSym = 1, HinAxis = 2 - 3, HinGroup = 3, 4, 5, 6, 7, 12)!!!! not corresponding to the correct hindered rotation.

HindrancePotential

theta	dE0 [kcal/mol]
-------	----------------

-153.6	0.0000
-143.6	0.0941
-133.6	0.3326
-123.6	0.6150
-113.6	0.8409
-103.6	0.9224
-93.6	0.8409
-83.6	0.6714
-73.6	0.4895
-63.6	0.3514
-53.6	0.2510
-43.6	0.2008
-33.6	0.1945
-23.6	0.2510
-13.6	0.3389
-3.6	0.4142
6.4	0.4079
16.4	0.3200
26.4	0.2322
36.4	0.1945
46.4	0.2134
56.4	0.2824
66.4	0.3891
76.4	0.5334
86.4	0.7154
96.4	0.8722
106.4	0.9099
116.4	0.7907
126.4	0.5397
136.4	0.2636
146.4	0.0565
156.4	0.0126
166.4	0.1757
176.4	0.5773
-173.6	0.4455
-163.6	0.1130
-153.6	0.0063

*!

Hindered Rotor = (HinMode = 4, HinSym = 3, HinAxis = 3 - 4, HinGroup = 4, 5, 6, 7)

HindrancePotential

theta dE0 [kcal/mol]

-171.2	0.0000
-161.2	0.0879
-151.2	0.2510
-141.2	0.4518
-131.2	0.6212
-121.2	0.7216
-111.2	0.7279
-101.2	0.6589
-91.2	0.5146
-81.2	0.3451
-71.2	0.1820
-61.2	0.0565
-51.2	0.0126
-41.2	0.0628
-31.2	0.2008
-21.2	0.3953
-11.2	0.5836
-1.2	0.7091
8.8	0.7342
18.8	0.6589
28.8	0.5020
38.8	0.3200
48.8	0.1443
58.8	0.0314
68.8	0.0063
78.8	0.0753
88.8	0.2196
98.8	0.4016
108.8	0.5773
118.8	0.6965
128.8	0.7342
138.8	0.6903
148.8	0.5522
158.8	0.3765
168.8	0.1883
178.8	0.0502
-171.2	0.0188

</IM1>

<TS-IM1-P1>

NAME TS3

Symmetry=1

Parity Undefined

OpticalIsomer=1

Tunneling=Eckart

EnergyLevel = (-381.292862, 1) !! hartree

Coordinates !! Angstrom

C	1.112141	0.032947	0.022519
O	0.213190	-0.703366	0.523458
C	-1.582791	-0.226865	0.049135
C	-1.560582	1.140706	0.309370
H	-1.210742	1.393770	1.306043
H	-0.301486	1.364651	-0.304202
H	-2.480935	1.637398	0.008497
C	2.530391	-0.472210	0.007517
H	2.643047	-1.308966	0.694433
H	2.767352	-0.808296	-1.005964
H	3.216883	0.336684	0.259165
O	-2.054562	-1.159992	-0.444769
O	0.887738	1.180519	-0.489841

FREQUENCY !! cm⁻¹

-1264.4245	50.2630	109.9489
117.3125	231.2695	332.4780
399.4623	484.4438	540.6296
605.4725	629.5278	651.1200
735.9589	896.2822	946.2848
1034.2462	1059.2173	1071.1431
1094.6413	1348.7452	1381.7787
1436.9645	1444.1322	1465.3068
1481.8267	1631.9854	1690.9969
2114.8392	3049.2071	3104.9863
3115.8799	3154.8262	3189.4298

Scale = 0.990

Hindered Rotor = (HinMode= 1, HinSym = 3, HinAxis = 1 - 8, HinGroup = 1, 2, 13)

HindrancePotential

theta	dE0 [kcal/mol]
-16.2	0.0000
-6.2	0.0063
3.8	0.0251
13.8	0.0502
23.8	0.0816
33.8	0.1130
43.8	0.1255
53.8	0.1255
63.8	0.1067
73.8	0.0690
83.8	0.0377
93.8	0.0126
103.8	0.0063
113.8	0.0126
123.8	0.0251
133.8	0.0439
143.8	0.0753

```

153.8      0.1004
163.8      0.1255
173.8      0.1318
-176.2     0.1130
-166.2     0.0690
-156.2     0.0314
-146.2     0.0126
-136.2     0.0000
-126.2     0.0063
-116.2     0.0251
-106.2     0.0502
-96.2      0.0753
-86.2      0.1004
-76.2      0.1192
-66.2      0.1255
-56.2      0.1130
-46.2      0.0816
-36.2      0.0439
-26.2      0.0188
-16.2      0.0000
</TS-IM1-P1>

<Outlet1>
Name CH3COOH !! acetic acid
Symmetry=1
Parity Undefined
OpticalIsomer=1
EnergyLevel = (-228.876671, 1) !! hartree
Coordinates !! Angstrom
C  -1.393668 -0.118247 -0.000145
H  -1.673680 -0.689689  0.887703
H  -1.671679 -0.713738 -0.872482
H  -1.919509  0.833508 -0.012818
C   0.091788  0.128191 -0.000415
O   0.785311 -1.038685 -0.000074
H   1.723837 -0.798731  0.001027
O   0.633729  1.202308  0.000065

FREQUENCY !! cm^-1
  68.1275      422.7331      544.5041
 587.4603      677.1123      860.8819
 997.8753     1068.4240     1211.1162
1344.2111     1409.1966     1473.1617
1476.5388     1838.8212     3051.7455
3111.4653     3161.5537     3759.6377
Scale = 0.990
Hindered Rotor = (HinMode = 1, HinSym = 3, HinAxis = 1 - 5, HinGroup = 1, 2, 3, 4)
HindrancePotential

```

theta	dE0 [kcal/mol]
-------	----------------

-179.3	0.0000
-169.3	0.0314
-159.3	0.1067
-149.3	0.2008
-139.3	0.2949
-129.3	0.3514
-119.3	0.3640
-109.3	0.3263
-99.3	0.2573
-89.3	0.1694
-79.3	0.0879
-69.3	0.0251
-59.3	0.0000
-49.3	0.0188
-39.3	0.0816
-29.3	0.1757
-19.3	0.2698
-9.3	0.3389
0.7	0.3702
10.7	0.3326
20.7	0.2573
30.7	0.1632
40.7	0.0753
50.7	0.0126
60.7	0.0000
70.7	0.0314
80.7	0.1004
90.7	0.1820
100.7	0.2698
110.7	0.3389
120.7	0.3640
130.7	0.3451
140.7	0.2824
150.7	0.1883
160.7	0.0941
170.7	0.0251
-179.3	0.0000

Hindered Rotor = (HinMode= 3, HinSym = 1, HinAxis = 5 - 6, HinGroup = 6, 7)

HindrancePotential

theta	dE0 [kcal/mol]
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-179.9	0.0000
-169.9	0.3389
-159.9	1.3742
-149.9	3.0497
-139.9	5.2146
-129.9	7.6368
-119.9	10.0339

-109.9	12.0984
-99.9	13.5291
-89.9	14.1315
-79.9	13.8993
-69.9	13.0208
-59.9	11.7407
-49.9	10.3225
-39.9	8.9546
-29.9	7.7937
-19.9	6.9152
-9.9	6.3818
0.1	6.1998
10.1	6.3818
20.1	6.9277
30.1	7.8125
40.1	8.9797
50.1	10.3414
60.1	11.7658
70.1	13.0334
80.1	13.9119
90.1	14.1315
100.1	13.5103
110.1	12.0670
120.1	9.9962
130.1	7.5929
140.1	5.1770
150.1	3.0183
160.1	1.3554
170.1	0.3326
-179.9	0.0000

</Outlet1>

<Outlet2>

Name CH2CO !!

Symmetry=2

Parity Undefined

OpticalIsomer=1

EnergyLevel = (-152.437005, 1) !! hartree

Coordinates !! Angstrom

C	0.000000	0.102507	0.000000
C	0.000000	-1.206955	0.000000
H	0.000000	-1.742012	0.938111
H	0.000000	-1.742012	-0.938111
O	0.000000	1.263839	0.000000

FREQUENCY !! cm⁻¹

447.5535	563.0297	596.1238
991.2414	1171.4639	1408.2804

2233.2067	3178.7006	3271.4000
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Scale = 0.990
</Outlet2>

<Product1>
Name CH₃COOH+CH₂CO
Components 1 2
</Product1>