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Role of Ring-Enlargement Reactions in the Formation of Aromatic Hydrocarbons

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1 Additional information on calibration

Information related to the species-specific parameters and the calibration procedure can be found in Table S1.

Table S1: Additional information on quantified species. M: nominal mass; IP: ionization potential [eV]; Ref. of *xs*: source of electron ionization cross section.

M	Species	Calibrated as	Calibration method	IP	Ref of *xs*
16	CH_4	Methane	Direct	12.61	[1]
26	C_2H_2	Acetylene	Direct	11.4	[2]
28	C_2H_4	Ethene	Direct	10.51	[3]
	CO	Carbon monoxide	Direct	14.01	[1]
30	CH_2O	Formaldehyde	Convolution	10.88	[4]
	C_2H_6	Ethane	Direct	11.52	[3]
32	O_2	Oxygen	Direct	12.07	[5]
42	C_2H_2O	Ketene	Convolution	9.62	[2]
	C_3H_6	Propene	Direct	9.73	[3]
50	C_4H_2	Buta-1,3-diyne	Convolution	9.58	[4]
52	C_4H_4	But-1-en-3-yne	Convolution	9.58	[4]
54	C_4H_6	1,3-Butadiene	Direct	9.07	[4]
56	C_4H_8	1-Butene	Direct	9.55	[4]
66	C_5H_6	1,3-Cyclopentadiene	Convolution	8.57	[2]
68	C_5H_8	cyclopentene	Direct	8.59	[2]
78	C_6H_6	Benzene	Direct	9.24	[4]
80	C_6H_8	Methylcyclopentadiene	Convolution	8.40	[2]
92	C_7H_8	Toluene	Direct	8.83	[2]
102	C_8H_6	Phenylacetylene	Convolution	8.82	[2]
104	C_8H_8	Styrene	Convolution	8.46	[2]
106	C_8H_{10}	Ethylbenzene	Convolution	8.76	[2]
116	C_9H_8	Indene	Convolution	8.14	[2]
128	$C_{10}H_8$	Naphthalene	Convolution	8.14	[2]

2 Quartz probe geometry

Figure S1 shows the technical details of the sampling quartz probe.

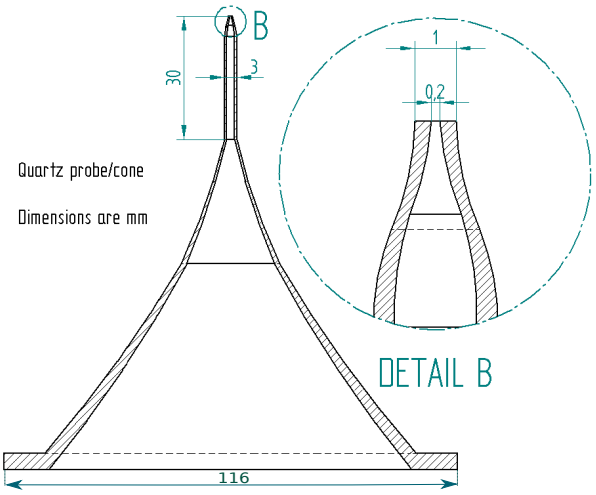


Figure S1: Technical drawing of the sampling nozzle. The figure is taken from Skeen et al. [6] where it is labeled as "Figure S2".

3 Summary of the modified reactions

In Table S2 the rate constants of the reactions which were updated or included in the CRECK$_{rev}$ model are reported. To facilitate the reader, Table S3 shows the chemical structures of some species which take part to some of these reactions but that are not introduced in the manuscript.

Table S2: List of reactions which have been updated or included in the CRECK$_{rev}$ model. Reactions (1)-(5) refer to the C_5H_6 updates; reactions (6)-(13) refer to the benzene and ethylbenzene subsets. The referenced papers are the source for the rate of each reaction.

	Reaction	A [$cm^3mol^{-1}s^{-1}$]	n	Ea [Cal mol^{-1}]	Ref.
(1)[1]	C_5H_6+H = a-C_3H_5+C_2H_2	3.8870E+28	-3.734	34872.00	[7]
(2)[1]	C_5H_6+H = C_5H_5+H_2	1.42E+07	2.091	3300.00	[7]
(3)[1]	C_5H_6+CH_3=C_5H_5+CH_4	2.78E+00	3.73	4701.60	This work
(4)[1]	C_5H_6+O=C_5H_5+OH	6.20E+06	2.12	4855.20	This work
(5)[1]	C_5H_6+OH=C_5H_5+H_2O	1.37E+04	4.10	-844.8	This work
(6)[1]	C_5H_6+HO_2=C_5H_5+H_2O_2	5.21E-03	4.23	9040.80	This work
(7)[2]	C_6H_6+H =C_6H_7#	3.2E+13	0.0	3200	[8]
(8)[2]	C_6H_7#+H=C_6H_8#	1.0E+14	0.0	0.0	[8]
(9)[2]	RMCPD=C_6H_7#	1.4E+13	0.0	17400	[8]
(10)[2]	MCPT+H=RMCPD+H_2	2.9E+07	2.0	7700	[8]
(11)[2]	RMCPDY=RMCPD	3.0E+12	0.0	50400	[8]
(12)[2]	MCPTD+H=RMCPDY+H_2	2.5E+04	2.5	-2700	[8]
(13)[2]	RMCPDY+H=MCPT	1.0E+14	0.0	0.0	[8]
(14)[2]	a-C_3H_5+C_5H_5=C_8H_{10}	5.0E+12	0.0	6000	[9]

[1] Reaction already included in the mechanism whose rate was updated according to the given reference.
[2] New reaction included in the mechanism the rate is given by the corresponding reference.

Table S3: Chemical structures

Formula	Structure	Formula	Structure
C_6H_7#		RMCPD	
C_6H_8		RMCPDY	

4 Additional comparisons

In this section some additional comparisons against available literature cases are shown to sensitivity to the newly updated C_5H_6 subset.

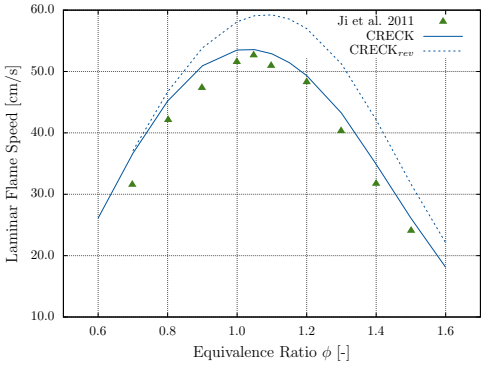


Figure S2: Comparison between the laminar burning velocity of C_5H_6 measured by Ji et al. [10] and the two versions of the CRECK model.

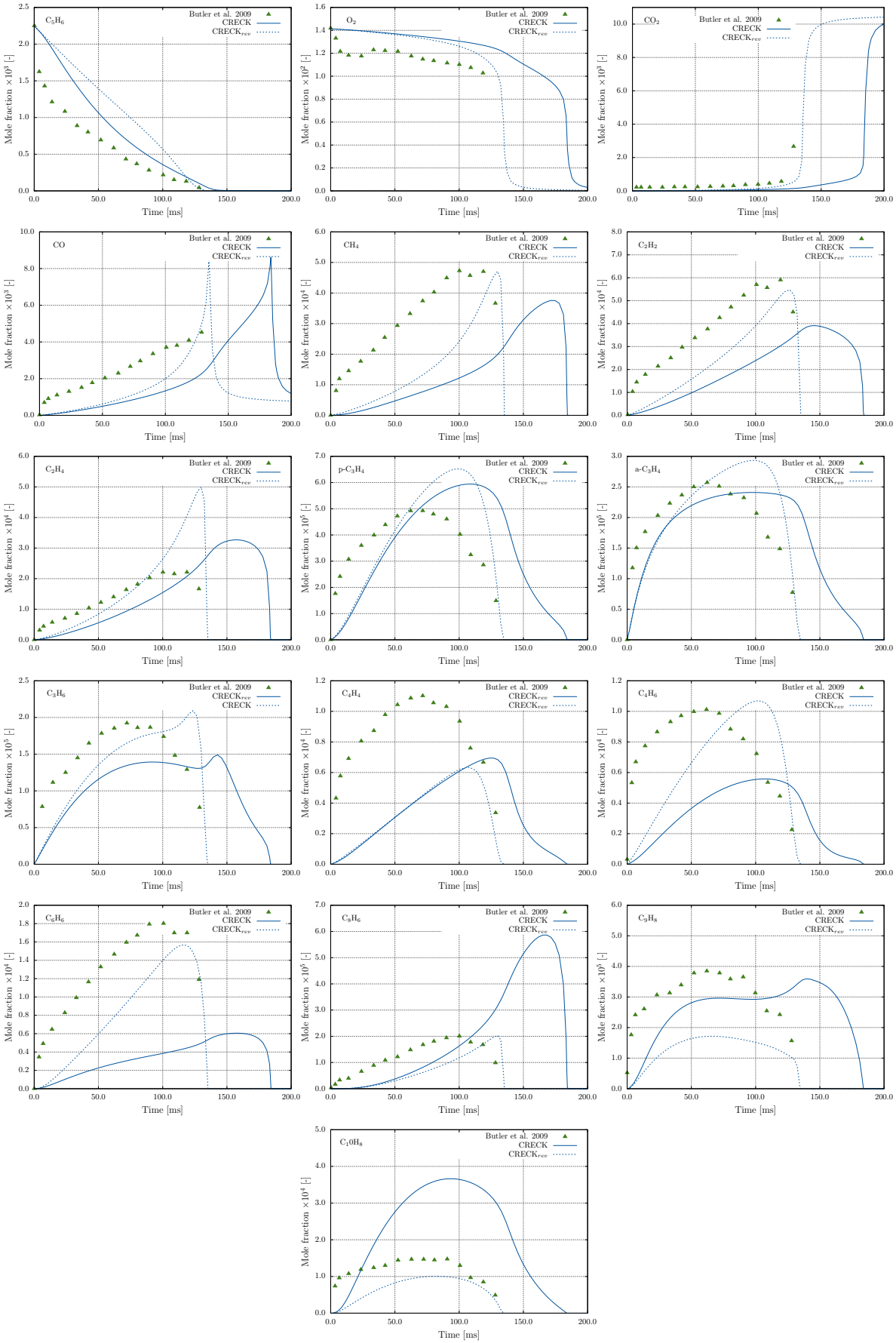


Figure S3: Comparison between the species mole fraction profiles measured by Butler et al. [11] and the two versions of the CRECK model. Here we refer to the oxidation case of the experimental study. Numerical results are not time-shifted.

5 Update on Gueniche model

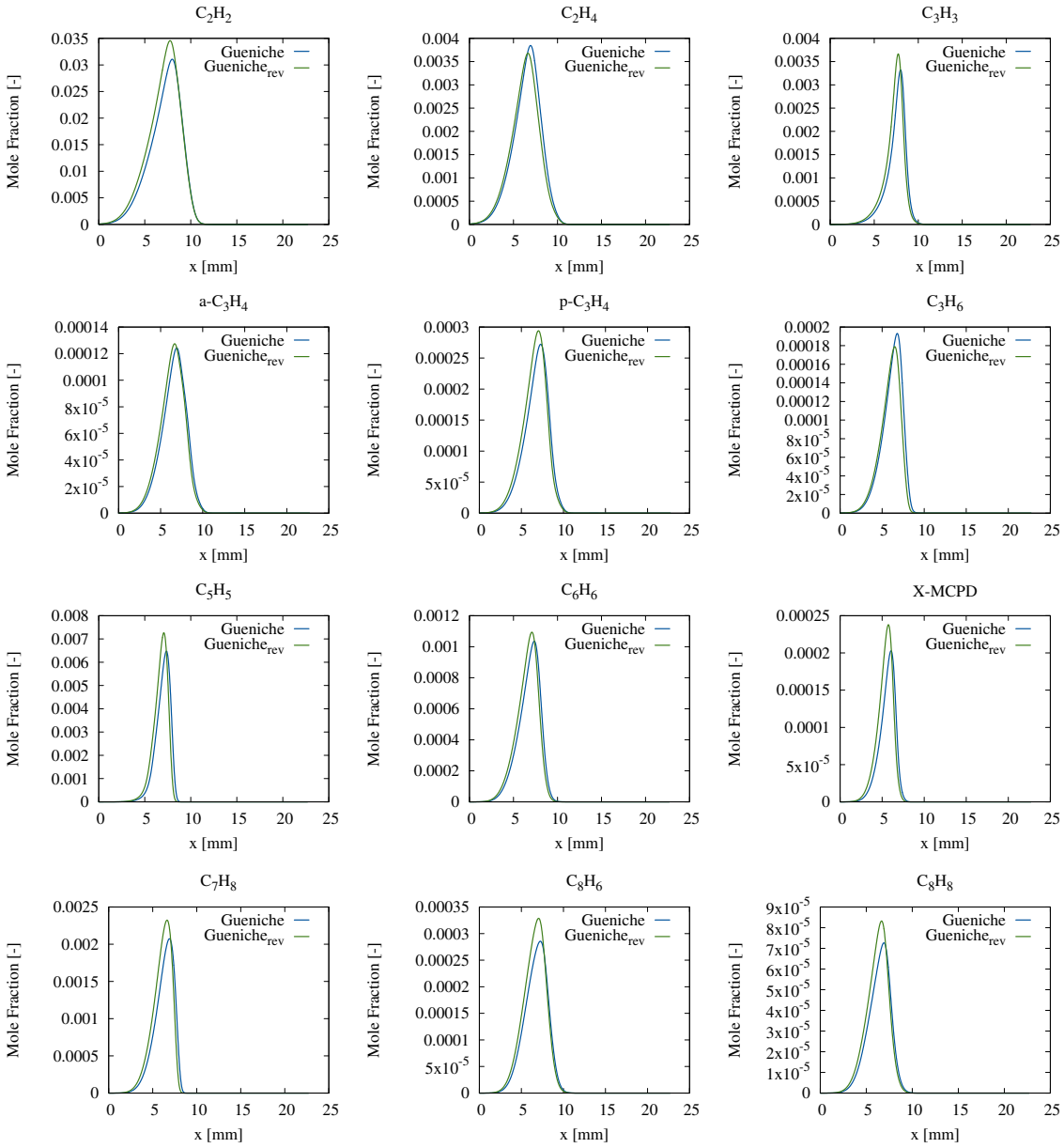


Figure S4: Comparison between the original version of the Gueniche model and the new one in which the new theoretically computed rates relative to H abstraction and addition to C_5H_6 were included (Gueniche$_{rev}$).

6 Spectrum for Flame$_{\mathrm{CPME}}$

Figure S5 shows the signal spectrum of Flame$_{\mathrm{CPME}}$ for comparison against Fig. 4 in the main manuscript which is related to Flame$_{\mathrm{CP}}$.

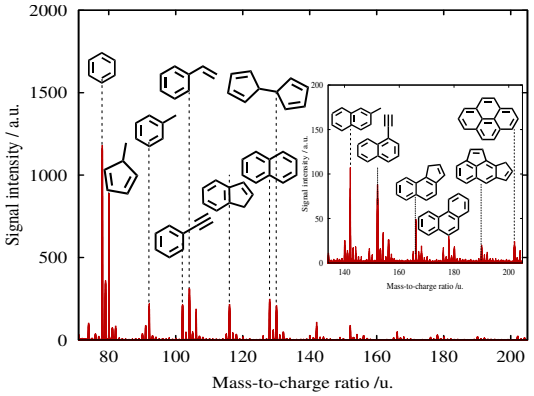


Figure S5: Signal mass spectrum obtained from $\text{Flame}_{\text{CPME}}$ at 8 mm from the fuel outlet.

7 Main species

Figure S6 depicts the measured and computed profiles of fuels, O_2, Ar, and major products for Flame_{CP} (a) and $\text{Flame}_{\text{CPME}}$ (b). In (a) and (b) symbols correspond to experimental results, solid lines to simulations performed with the Gueniche model, and dashed lines to the CRECK model. The computed temperature profile is also included. The axial coordinate x represents the distance from the fuel inlet.

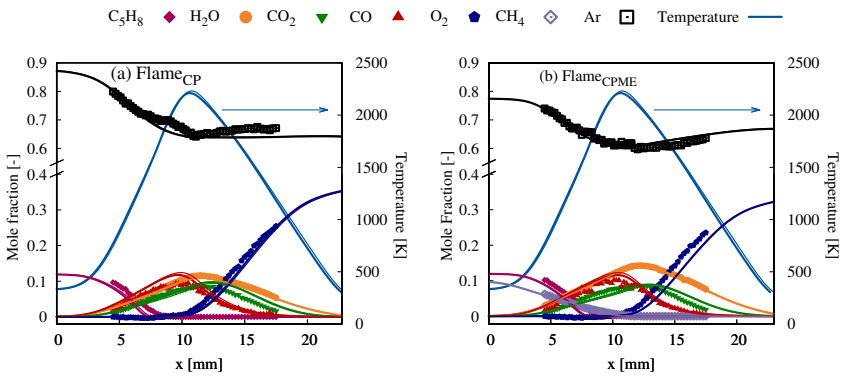


Figure S6: Left y-axis: comparison between the measured and computed mole fraction of the fuels C_5H_8 and CH_4, O_2, CO, CO_2, H_2O and argon; right y-axis: computed temperature profile. The axial coordinate x represents the distance from the fuel outlet

8 Species profiles for $\text{Flame}_{\text{CPME}}$

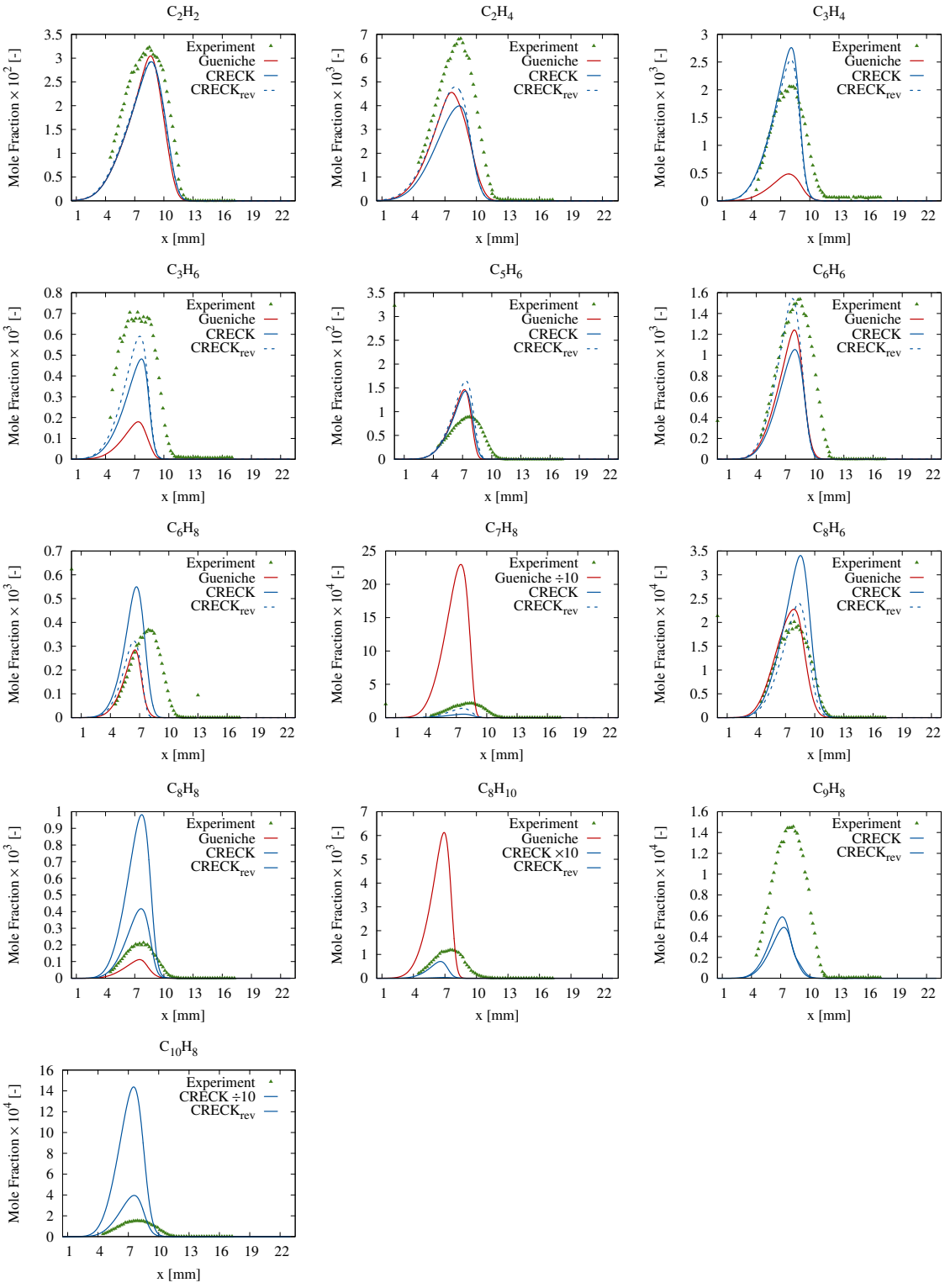


Figure S7: Comparison between the computed and measured mole fractions for flame $\text{Flame}_{\text{CPME}}$. The axial coordinate x represents the distance from the fuel inlet.

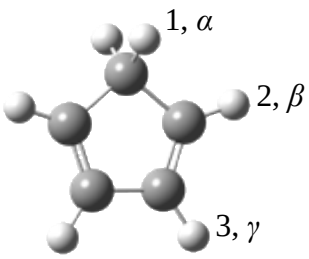
9 Quantum chemistry calculations

Table S4. T1 diagnostic for species calculated at CCSD(T)/cc-pVTZ

species	T1 DIAG
CH3	0.0078978
O	0.0053117
OH	0.0070486
HO2	0.0269716
C5H6	0.011011
C5H6_CH3_TS_1	0.015178
C5H6_CH3_TS_2	0.042166
C5H6_CH3_TS_3	0.04209690
C5H6_O_RC_1	0.0127246
C5H6_O_RC_2	0.0127246
C5H6_O_RC_3	0.0127647
C5H6_O_TS_1	0.0423394
C5H6_O_TS_2	0.0437105
C5H6_O_TS_3	0.0431695
C5H6_O_PC_1	0.02409635
C5H6_O_PC_2	0.0437105
C5H6_O_PC_3	0.04237754
C5H6_HO2_RC_1	0.0193136
C5H6_HO2_RC_2	0.0193236
C5H6_HO2_RC_3	0.0192997
C5H6_HO2_TS_1	0.0379489
C5H6_HO2_TS_2	0.0408391
C5H6_HO2_TS_3	0.0405671
C5H6_HO2_PC_1	0.0251884
C5H6_HO2_PC_2	0.0384445
C5H6_HO2_PC_3	0.0383216
C5H6_OH_RC_1	0.0138952
C5H6_OH_RC_2	0.0139031
C5H6_OH_RC_3	0.0139005
C5H6_OH_TS_1	0.0400587
C5H6_OH_TS_2	0.0432501
C5H6_OH_TS_3	0.025314
C5H6_OH_PC_1	0.0266282
C5H6_OH_PC_2	0.0416137
C5H6_OH_PC_3	0.04171202
C5H5_1	0.03076478
C5H5_2	0.04356202
C5H5_3	0.04360555
CH4	0.0072118
H2O2	0.0096535
H2O	0.0065206

Table S5. CCSD(T)/cc-pVDZ, CCSD(T)/cc-pVTZ and CCSD(T)/CBS energies of stationary points (unit: Hartrees)

	CCSD(T)/cc-pVDZ_HF	CCSD(T)/cc-pVDZ	CCSD(T)/cc-pVTZ_HF	CCSD(T)/cc-pVDZ	CCSD(T)/CBS
H	-0.499278	-0.499278	-0.499810	-0.499810	-0.499989
C5H6	-192.808652	-193.543895	-192.858119	-193.735882	-193.839118
C5H6_H_TS	-193.280720	-194.029146	-193.330392	-194.223223	-194.327674
C5H5	-192.210472	-192.906230	-192.258469	-193.092768	-193.193091
H2	-1.128703	-1.163382	-1.132966	-1.172333	-1.176617
CH3	-39.563808	-39.715835	-39.577471	-39.760976	-39.784700
C5H6	-192.808652	-193.543895	-192.858119	-193.735882	-193.839118
C5H6_CH3_TS	-232.337245	-233.243984	-232.398760	-233.481821	-233.609648
CH4	-40.198706	-40.387088	-40.213330	-40.438099	-40.465128
C5H5	-192.210472	-192.906230	-192.258469	-193.092768	-193.193091
O	-74.792166	-74.909950	-74.811757	-74.973962	-75.007544
C5H6	-192.808652	-193.543895	-192.858119	-193.735882	-193.839118
C5H6_O_RC	-267.594616	-268.455207	-267.662414	-268.712125	-268.849842
C5H6_O_TS	-267.561022	-268.431838	-267.629491	-268.692450	-268.832229
C5H6_O_PC	-267.599470	-268.471086	-267.671446	-268.737288	-268.879514
C5H5	-192.210472	-192.906230	-192.258469	-193.092768	-193.193091
OH	-75.393787	-75.559304	-75.419172	-75.637723	-75.678488
HO2	-150.187909	-150.557772	-150.237198	-150.712034	-150.792402
C5H6	-192.808652	-193.543895	-192.858119	-193.735882	-193.839118
C5H6_HO2_RC	-343.000241	-344.112743	-343.097122	-344.458783	-344.642767
C5H6_HO2_TS	-342.939513	-344.073780	-343.035369	-344.421949	-344.607503
C5H6_HO2_PC	-342.997534	-344.107907	-343.095477	-344.458892	-344.645592
C5H5	-192.210472	-192.906230	-192.258469	-193.092768	-193.193091
H2O2	-150.785601	-151.192905	-150.837692	-151.357928	-151.444073
OH	-75.393787	-75.559304	-75.419172	-75.637723	-75.678488
C5H6	-192.808652	-193.543895	-192.858119	-193.735882	-193.839118
C5H6_OH_RC	-268.201576	-269.109675	-268.274675	-269.380202	-269.524752
C5H6_OH_TS	-268.180864	-269.096225	-268.254204	-269.368718	-269.514396
C5H6_OH_PC	-268.239419	-269.154172	-268.316358	-269.431964	-269.579887
C5H5	-192.210472	-192.906230	-192.258469	-193.092768	-193.193091
H2O	-76.026684	-76.240983	-76.057056	-76.332156	-76.379319



c-C_5H_6

Figure. S10. Molecular structure of C_5H_6

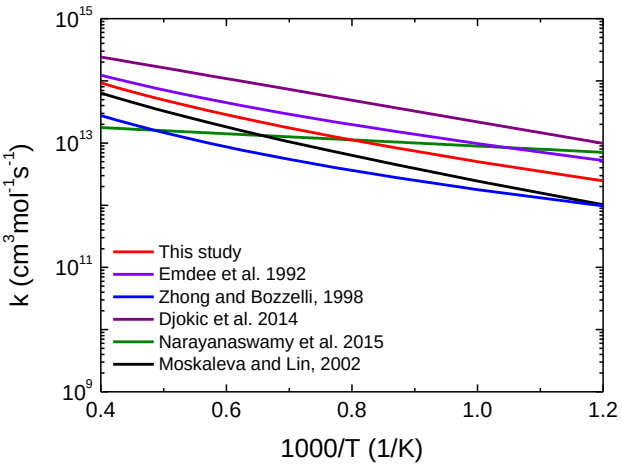


Figure S11. HPL rate constants for hydrogen abstraction reaction of C_5H_6 by H atom

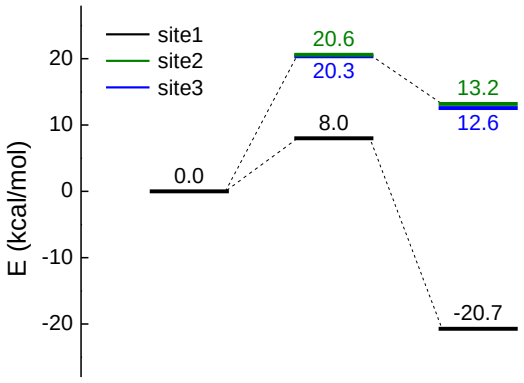


Figure. S12. Potential energy surface (PES) of hydrogen abstraction of C_5H_6 by CH_3 at the CCSD(T)-CBS//M06-2X/6-311+G(d,p) level of theory (in kcal/mol).

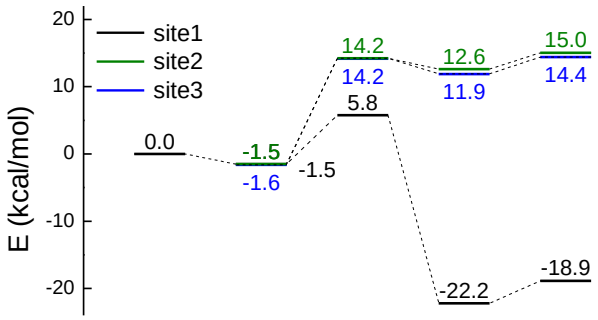


Figure. S13. Potential energy surface (PES) of hydrogen abstraction of C_5H_6 by $O(^3P)$ at the CCSD(T)-CBS//M06-2X/6-311+G(d,p) level of theory (in kcal/mol).

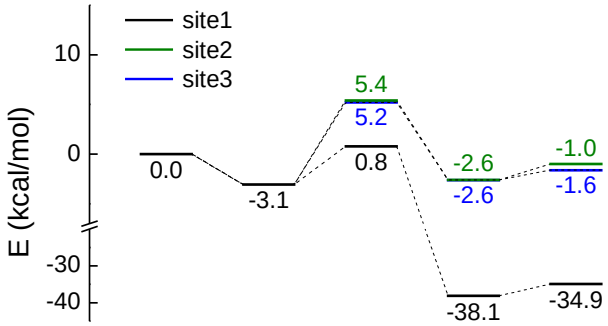


Figure. S14 Potential energy surface (PES) of hydrogen abstraction of C_5H_6 by OH at the CCSD(T)-CBS//M06-2X/6-311+G(d,p) level of theory (in kcal/mol).

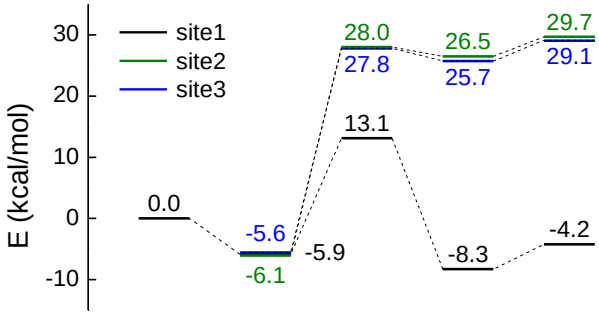


Figure. S15 Potential energy surface (PES) of hydrogen abstraction of C_5H_6 by HO_2 at the CCSD(T)-CBS//M06-2X/6-311+G(d,p) level of theory (in kcal/mol).

```
!****************************************************
!            GLOBAL SECTION, MESS for c-C5H6+O
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]                  300 400 500 600 700 773 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800
1900 2000 2100 2200 2300 2400 2500
PressureList[atm]                   0.01 0.1 1 10 100
!
!** Methods **
```

CalculationMethod direct ! direct or low-eigenvalue
ReductionMethod diagonalization ! threshold (default), sort_out (most accurate but costly), incremental, sequential
WellProjectionThreshold 0.2 ! default=0.2
!!!!REMOVED!!!!LowEigenvalueRateReductionMethod projection ! [low eigenvalue method only] diagonalization or projection (default)
!** Grids **
EnergyStepOverTemperature .2 ! [Discretization energy step (global relax matrix)] / T
ExcessEnergyOverTemperature 30 ! [Highest barrier in the model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol] 400 ! Highest reference energy used in the calculation (or ReferenceEnergy[kcal/mol])
!!
!** Cutoff **
WellCutoff 20 ! well truncation parameter : Max { dissociation limit (min barrier rel. to bottom of the well) / T }
ChemicalEigenvalueMax 0.2 ! Max chemical eigenvalue / Lowest Collision relaxation eigenvalue
ChemicalEigenvalueMin 1e-6 ! [Min chemical eigenvalue / Lowest Collision relaxation eigenvalue] for which direct method is used
AtomDistanceMin[bohr] 1.5 ! minimal interatomic distance (geometry checking)
!
!** Reference energy **
Reactant r0 ! Bimolecular species whose ground energy will be used as a reference for energy
!!** Outputs **
EigenvalueOutput Rxn1eg.out
RateOutput Rxn1.out
LogOutput Rxn1.log
!
MicroEnerMin[kcal/mol] 0.
MicroEnerMax[kcal/mol] 20.
MicroEnerStep[kcal/mol] 0.1
!
!
!!!
!**
! MODEL SECTION
!**
!!!
!
!
Model
!
EnergyRelaxation ! Default collisional energy relaxation kernel
Exponential ! Currently the only possible energy relaxation model
Factor[1/cm] 400 ! (Delta_E_down)^(0) @ standard T (300 K)
Power 0.7 ! Power n in the expression (Delta_E_down) = (Delta_E_down)^(0)

```
(T/T0)^(n)
      ExponentCutoff                10                        ! if (Delta_E) / (Delta_E_down) > value  transition probability is zero
   End
!
  CollisionFrequency                                        ! Collision frequency model
    LennardJones                                           ! Currently the only possible collisional frequency model  based on LJ
potential
      Epsilons[1/cm]                  273.8  79.23              ! Epsilon_1 and Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K
= x 1.4) Ar and C5H5 (from Lindstedt et al )
      Sigmas[angstrom]                 5.78   3.47               ! Sigma_1 and Sigma_2 (from Lindstedt et al )
      Masses[amu]                      82      39.948            ! Masses of the buffer gas molecule and of the complex (check
order)
   End
!
!************************************************
!**********************************
 Well RC
 Species
 RRHO     ! fake well
 Geometry[angstrom]            12
 C              -0.55567900   -1.17368000   -0.05220500
 C               0.11043400   -0.73324900    1.03283200
 C               0.11043200    0.73325200    1.03283100
 C              -0.55568200    1.17367900   -0.05220800
 H              -0.72110000   -2.20520900   -0.33019900
 H               0.58683300   -1.34834200    1.78403900
 H               0.58682900    1.34834800    1.78403600
 H              -0.72110600    2.20520700   -0.33020400
 C              -1.06696900   -0.00000200   -0.83495300
 H              -0.69409900   -0.00000300   -1.86429600
 H              -2.16263100   -0.00000400   -0.88883300
 O               1.85875600    0.00000100   -0.86404100
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            SymmetryFactor    1
       End
Frequencies[1/cm]          30
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120.116846
154.436028
333.324398
506.369779
664.248046
714.466983
789.473203
793.601038
888.695958
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911.465447
936.285904
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1108.057093
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1285.534016
1357.123799
1373.573059
1522.156883
1597.137883
2966.515692
3007.910927
3136.680658
3144.442113
3159.567032
3166.228895
 ZeroEnergy[kcal/mol]           -1.6
 ElectronicLevels[1/cm]          1
    0.0                  3
End
End
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!  REACTANTS
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
 Bimolecular REACS
 Fragment REACT1
 RRHO
 Geometry[angstrom]             11
 C              0.00015600   -0.28081200    1.17594600
 C              0.00015600    0.98779800    0.73475200
 C              0.00015600    0.98779800   -0.73475200
 C              0.00015600   -0.28081200   -1.17594600
 H              0.00019600   -0.60649500    2.20697000
 H              0.00032600    1.87799900    1.35003400
 H              0.00032600    1.87799900   -1.35003400
 H              0.00019600   -0.60649500   -2.20697000
 C             -0.00053900   -1.21425500    0.00000000
 H              0.87792900   -1.87097300    0.00000000
```

```
 H               -0.87948000   -1.87034400    0.00000000
       Core         RigidRotor
            SymmetryFactor    2.00000000000000
       End
    Frequencies[1/cm]          27
332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
 0.000000000000000E+000   1.00000000000000
End
!***********************************
Fragment REACT2
 Atom
 Name O
 ElectronicLevels[1/cm]                  3
 0.000000000000000E+000   5.00000000000000
  158.300000000000        3.00000000000000
  226.000000000000        1.00000000000000
End
GroundEnergy[kcal/mol] 0.0
```

```
End
!************************************************
!!!!  PRODUCTS            !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
Bimolecular ProdS
Fragment Prod1
RRHO
Geometry[angstrom]             10
C              -0.00007800   -0.35099600    1.16853400
C              -0.00007800    0.94378900    0.73860100
C              -0.00007800    0.94378900   -0.73860100
C              -0.00007800   -0.35099600   -1.16853400
H               0.00038200   -0.69970600    2.18955800
H               0.00125900    1.83135400    1.35549300
H               0.00125900    1.83135400   -1.35549300
H               0.00038200   -0.69970600   -2.18955800
C              -0.00010300   -1.18505500    0.00000000
H              -0.00079100   -2.26648000    0.00000000
      Core        RigidRotor
           SymmetryFactor    10.00000000000000
      End
   Frequencies[1/cm]          24
328.999168
489.124246
508.641713
682.343299
725.107204
814.03079
819.329512
894.783969
907.829111
910.64279
934.474138
1035.7175
1050.867445
1120.71666
1193.86533
1255.526193
1355.146163
1475.063286
1511.608909
3127.261085
3143.895518
3152.533174
3164.305967
3172.474628
```

```
 ZeroEnergy[kcal/mol]             0.0
 ElectronicLevels[1/cm]                   1
 0.000000000000000E+000   2.00000000000000
End
!***********************************
Fragment Prod2
 RRHO
 Geometry[angstrom]             2
 O                0.00000000    0.00000000    0.10800300
 H                0.00000000    0.00000000   -0.86402400
       Core        RigidRotor
            SymmetryFactor    1.00000000000000
       End
    Frequencies[1/cm]          1
3653.178498
 ZeroEnergy[kcal/mol]             0.0
 ElectronicLevels[1/cm]                   1
   0.000000000000        2.00000000000000
End
GroundEnergy[kcal/mol] -18.9
End
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***********************************
 Barrier B1 REACS RC
 RRHO
 Stoichiometry  C5H6O1
 Core  PhaseSpaceTheory
 FragmentGeometry[angstrom]   11
 C                0.00015600   -0.28081200    1.17594600
 C                0.00015600    0.98779800    0.73475200
 C                0.00015600    0.98779800   -0.73475200
 C                0.00015600   -0.28081200   -1.17594600
 H                0.00019600   -0.60649500    2.20697000
 H                0.00032600    1.87799900    1.35003400
 H                0.00032600    1.87799900   -1.35003400
 H                0.00019600   -0.60649500   -2.20697000
 C               -0.00053900   -1.21425500    0.00000000
 H                0.87792900   -1.87097300    0.00000000
 H               -0.87948000   -1.87034400    0.00000000
 FragmentGeometry[angstrom]   1
 O                0.00000000    0.00000000    0.00000000
 SymmetryFactor    1.0000000000000000
 PotentialPrefactor[au] 48.7
 PotentialPowerExponent  6
 End
 Frequencies[1/cm]          27
```

332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
ZeroEnergy[kcal/mol] 0
ElectronicLevels[1/cm] 3
0.0000000000000000 5.0000000000000000
158.30000000000001 3.0000000000000000
226.00000000000000 1.0000000000000000
End
!**********
Barrier B2 RC ProdS
RRHO
Geometry[angstrom] 12
C -0.27249900 1.15588100 0.35712300
C -1.35393900 0.80532400 -0.36264600
C -1.44421800 -0.66384500 -0.41646700
C -0.41501700 -1.19595500 0.26883300
H 0.07286000 2.15564000 0.57555100
H -2.05553400 1.48134800 -0.83215600
H -2.22196700 -1.21252200 -0.93017700
H -0.19704600 -2.24399700 0.41182200
C 0.42538600 -0.08570100 0.78536300

```
 H              1.43564600   -0.10670900    0.12115700
 H              0.80936000   -0.14575400    1.80356100
 O              2.56480100   -0.00277800   -0.61787400
   Core     RigidRotor
         SymmetryFactor    1.0000000000000000
   End
   Tunneling    Eckart
     ImaginaryFrequency[1/cm]    1066.712492
     WellDepth[kcal/mol]          7.4
     WellDepth[kcal/mol]          24.7
   End
   Frequencies[1/cm]    29
75.219329
103.837724
376.958005
514.246276
667.868086
698.143823
723.480126
773.605846
798.885695
872.309845
925.11228
935.377208
945.747187
955.226512
998.779027
1033.792147
1078.756982
1104.543365
1198.651989
1232.319622
1278.625579
1362.374894
1525.828527
1587.657006
3044.219191
3122.575985
3136.889014
3148.928945
3158.70509
  ZeroEnergy[kcal/mol]    5.8
  ElectronicLevels[1/cm]                  2
   0.0000000000000000       3.0000000000000000
   114.20000000000000       3.0000000000000000
End
```

```
!
!
!

!************************************************
!               END OF INPUT
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
End


!************************************************
!             GLOBAL SECTION , MESS for c-C5H6+OH
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]                  300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900
2000 2100 2200 2300 2400 2500
PressureList[atm]                   0.01 0.1 1 10 100
!
!** Methods **
CalculationMethod                   direct                      ! direct or low-eigenvalue
ReductionMethod                     diagonalization                 ! threshold (default), sort_out (most accurate but costly),
incremental, sequential
WellProjectionThreshold             0.2                         ! default=0.2
!!!!REMOVED!!!!LowEigenvalueRateReductionMethod      projection                  ! [low eigenvalue method only]
diagonalization or projection (default)
!**  Grids  **
EnergyStepOverTemperature           .2      ! [Discretization energy step (global relax matrix)] / T
ExcessEnergyOverTemperature         30      ! [Highest barrier in the model (global relax matrix)] / T
ModelEnergyLimit[kcal/mol]                  400             ! Highest reference energy used in the calculation ( or
ReferenceEnergy[kcal/mol])
!!
!** Cutoff  **
WellCutoff                      20      ! well truncation parameter : Max { dissociation limit (min barrier rel. to bottom of
the well) / T }
ChemicalEigenvalueMax               0.2     ! Max chemical eigenvalue / Lowest Collision relaxation eigenvalue
ChemicalEigenvalueMin               1e-6                        ! [Min chemical eigenvalue / Lowest Collision relaxation
eigenvalue] for which direct method is used
AtomDistanceMin[bohr]               1.5                         ! minimal interatomic distance (geometry checking)
!
!** Reference energy **
Reactant                        r0                      ! Bimolecular species whose ground energy will be used as a reference
for energy
```

```
!!** Outputs **
EigenvalueOutput                Rxn1eg.out
RateOutput                      Rxn1.out
LogOutput                       Rxn1.log
!
MicroEnerMin[kcal/mol]           0.
MicroEnerMax[kcal/mol]           20.
MicroEnerStep[kcal/mol]          0.1
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***********************************************
!            MODEL SECTION
!***********************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
 EnergyRelaxation                          ! Default collisional energy relaxation kernel
  Exponential                             ! Currently the only possible energy relaxation model
    Factor[1/cm]              400           ! (Delta_E_down)^(0) @ standard T (300 K)
    Power                     0.7           ! Power n in the expression (Delta_E_down) = (Delta_E_down)^(0)
(T/T0)^(n)
    ExponentCutoff            10            ! if (Delta_E) / (Delta_E_down) > value  transition probability is zero
  End
!
 CollisionFrequency                        ! Collision frequency model
  LennardJones                            ! Currently the only possible collisional frequency model  based on LJ
potential
    Epsilons[1/cm]            273.8  79.23        ! Epsilon_1 and Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K
= x 1.4) Ar and C5H5 (from Lindstedt et al )
    Sigmas[angstrom]           5.78   3.47        ! Sigma_1 and Sigma_2 (from Lindstedt et al )
    Masses[amu]               82      39.948      ! Masses of the buffer gas molecule and of the complex (check
order)
  End
!
!***********************************************
!*********************************
 Well RC
 Species
 RRHO    ! fake well
 Geometry[angstrom]          13
 C            -0.17492000    0.29421800    1.12356400
 C             0.11674900   -0.97912200    0.79249400
 C             0.97289200   -0.97978100   -0.40127300
```

```
 C             1.19562000    0.29114000   -0.78561900
 H            -0.79494700    0.61879100    1.94692000
 H            -0.22965900   -1.86686400    1.30392100
 H             1.35841300   -1.86943100   -0.88143900
 H             1.79456700    0.61336400   -1.62615200
 C             0.50415800    1.22625700    0.16444500
 H            -0.21244000    1.88525200   -0.33735800
 H             1.22661400    1.87267400    0.67803500
 O            -2.17715200    0.00020100   -0.66370100
 H            -1.41232700   -0.37166500   -1.13598800
      Core        RigidRotor
           SymmetryFactor    1
      End
Frequencies[1/cm]          33
73.715053
102.309295
148.669863
304.14641
338.682581
475.85581
512.937358
667.739852
720.032746
791.806635
795.653655
888.681505
915.272891
934.922472
950.779159
951.765552
991.915986
1079.616984
1098.783117
1099.520899
1235.188494
1287.928655
1358.850593
1376.02066
1523.717128
1602.087696
2953.453575
2995.408015
3113.832793
3123.791007
3142.512686
3148.914977
```

```
3633.245289
 ZeroEnergy[kcal/mol]           -3.1
 ElectronicLevels[1/cm]          1
    0.0                  2
End
End
!**************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!**************************************************
!  REACTANTS
!**************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!**************************************************
 Bimolecular REACS
 Fragment REACT1
 RRHO
 Geometry[angstrom]             11
 C              0.00015600   -0.28081200    1.17594600
 C              0.00015600    0.98779800    0.73475200
 C              0.00015600    0.98779800   -0.73475200
 C              0.00015600   -0.28081200   -1.17594600
 H              0.00019600   -0.60649500    2.20697000
 H              0.00032600    1.87799900    1.35003400
 H              0.00032600    1.87799900   -1.35003400
 H              0.00019600   -0.60649500   -2.20697000
 C             -0.00053900   -1.21425500    0.00000000
 H              0.87792900   -1.87097300    0.00000000
 H             -0.87948000   -1.87034400    0.00000000
      Core        RigidRotor
           SymmetryFactor    2.00000000000000
      End
   Frequencies[1/cm]          27
332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
```

```
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
 0.000000000000000E+000   1.00000000000000
End
!***********************************
Fragment REACT2
 RRHO
 Geometry[angstrom]             2
 O               0.00000000    0.00000000    0.10800300
 H               0.00000000    0.00000000   -0.86402400
       Core        RigidRotor
             SymmetryFactor    1.00000000000000
       End
    Frequencies[1/cm]          1
3653.178498
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  2
 0.000000000000000E+000   2.00000000000000
  140.000000000000        2.00000000000000
End
GroundEnergy[kcal/mol] 0.0
End
!************************************************
!!!!  PRODUCTS             !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
 Bimolecular ProdS
 Fragment Prod1
 RRHO
 Geometry[angstrom]             10
 C              -0.00007800   -0.35099600    1.16853400
 C              -0.00007800    0.94378900    0.73860100
 C              -0.00007800    0.94378900   -0.73860100
 C              -0.00007800   -0.35099600   -1.16853400
```

```
 H              0.00038200   -0.69970600    2.18955800
 H              0.00125900    1.83135400    1.35549300
 H              0.00125900    1.83135400   -1.35549300
 H              0.00038200   -0.69970600   -2.18955800
 C             -0.00010300   -1.18505500    0.00000000
 H             -0.00079100   -2.26648000    0.00000000
      Core        RigidRotor
           SymmetryFactor    10.00000000000000
      End
   Frequencies[1/cm]          24
328.999168
489.124246
508.641713
682.343299
725.107204
814.03079
819.329512
894.783969
907.829111
910.64279
934.474138
1035.7175
1050.867445
1120.71666
1193.86533
1255.526193
1355.146163
1475.063286
1511.608909
3127.261085
3143.895518
3152.533174
3164.305967
3172.474628
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
 0.000000000000000E+000   2.00000000000000
End
!***********************************
Fragment Prod2 !H2O
 RRHO
 Geometry[angstrom]             3
 O              0.00000000    0.00000000    0.11656500
 H              0.00000000   -0.76161600   -0.46625800
 H              0.00000000    0.76161600   -0.46625800
      Core        RigidRotor
```

```
            SymmetryFactor    2.00000000000000
       End
    Frequencies[1/cm]          3
1547.361266
3779.007577
3881.837956
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
    0.000000000000        1.00000000000000
 End
 GroundEnergy[kcal/mol] -34.9
 End
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!**********************************
 Barrier B1 REACS RC
 RRHO
 Stoichiometry  C5H7O1
 Core  PhaseSpaceTheory
 FragmentGeometry[angstrom]   11
 C              0.00015600   -0.28081200    1.17594600
 C              0.00015600    0.98779800    0.73475200
 C              0.00015600    0.98779800   -0.73475200
 C              0.00015600   -0.28081200   -1.17594600
 H              0.00019600   -0.60649500    2.20697000
 H              0.00032600    1.87799900    1.35003400
 H              0.00032600    1.87799900   -1.35003400
 H              0.00019600   -0.60649500   -2.20697000
 C             -0.00053900   -1.21425500    0.00000000
 H              0.87792900   -1.87097300    0.00000000
 H             -0.87948000   -1.87034400    0.00000000
 FragmentGeometry[angstrom]   2
 O              0.00000000    0.00000000    0.10800300
 H              0.00000000    0.00000000   -0.86402400
 SymmetryFactor    1.0000000000000000
 PotentialPrefactor[au] 73.8
 PotentialPowerExponent  6
 End
 Frequencies[1/cm]          28
332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
```

953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
3653.178498
ZeroEnergy[kcal/mol] 0
ElectronicLevels[1/cm] 2
0.0000000000000000 2.0000000000000000
140.00000000000000 2.0000000000000000
End
!**********
Barrier B2 RC ProdS
RRHO
Geometry[angstrom] 13
C -0.29553000 1.13319100 0.42538900
C -1.33844000 0.84376100 -0.37251700
C -1.46789400 -0.61888300 -0.48620600
C -0.50090800 -1.20601000 0.24191600
H 0.06056100 2.11435100 0.70481900
H -1.98966900 1.55795100 -0.85827300
H -2.22751200 -1.12544500 -1.06625100
H -0.32421300 -2.26558600 0.35672500
C 0.34087400 -0.14529400 0.86367100
H 1.41112800 -0.20529900 0.40161600
H 0.53611600 -0.24509000 1.93438700
O 2.51548800 -0.02248100 -0.52944100
H 1.98107000 0.30837900 -1.27101400
Core RigidRotor
SymmetryFactor 1.0000000000000000
End
Rotor Hindered

Group 13
Axis 10 12
Symmetry 1
Potential[kcal/mol] 15
0.1388805
0.093361554
0.030723
0
0.1665939
0.4824138
0.6059328
0.4824138
0.1665939
0
0.030723
0.093361554
0.1388805
0.1702305
0.169917
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 986.089099
WellDepth[kcal/mol] 3.9
WellDepth[kcal/mol] 35.7
End
Frequencies[1/cm] 31
71.517615
208.943432
304.436149
508.921364
636.856022
711.394314
734.292716
784.975992
798.227065
851.508486
909.054027
923.157536
938.372762
942.582271
994.62345
1009.80589
1078.22193
1100.586638
1218.15219
1239.629833

```
1283.536689
1364.222647
1459.211643
1532.509499
1598.624117
3010.91298
3114.465718
3125.821896
3145.649763
3150.665148
3654.645138
 ZeroEnergy[kcal/mol]    0.8
 ElectronicLevels[1/cm]                  1
 0.0000000000000000         2.0000000000000000
End

!
!
!

!****************************************************
!               END OF INPUT
!****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
End

!************************************************
!             GLOBAL SECTION,MESS for c-C5H6+HO2
!************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
TemperatureList[K]                  300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900
2000 2100 2200 2300 2400 2500
PressureList[atm]                  0.01 0.1 1 10 100
!
!** Methods **
CalculationMethod                   direct                          ! direct or low-eigenvalue
ReductionMethod                     diagonalization                       ! threshold (default), sort_out (most accurate but costly),
incremental, sequential
WellProjectionThreshold             0.2                             ! default=0.2
!!!!REMOVED!!!!LowEigenvalueRateReductionMethod      projection                      ! [low eigenvalue method only]
diagonalization or projection (default)
!**  Grids  **
EnergyStepOverTemperature           .2        ! [Discretization energy step (global relax matrix)] / T
ExcessEnergyOverTemperature         30        ! [Highest barrier in the model (global relax matrix)] / T
```

```
ModelEnergyLimit[kcal/mol]                400          ! Highest reference energy used in the calculation ( or
ReferenceEnergy[kcal/mol])
!!
!** Cutoff  **
WellCutoff                    20      ! well truncation parameter : Max { dissociation limit (min barrier rel. to bottom of
the well) / T }
ChemicalEigenvalueMax         0.2     ! Max chemical eigenvalue / Lowest Collision relaxation eigenvalue
ChemicalEigenvalueMin         1e-6                ! [Min chemical eigenvalue / Lowest Collision relaxation
eigenvalue] for which direct method is used
AtomDistanceMin[bohr]         1.5                 ! minimal interatomic distance (geometry checking)
!
!** Reference energy **
Reactant                      r0                  ! Bimolecular species whose ground energy will be used as a reference
for energy
!!** Outputs **
EigenvalueOutput              Rxn1eg.out
RateOutput                    Rxn1.out
LogOutput                     Rxn1.log
!
MicroEnerMin[kcal/mol]        0.
MicroEnerMax[kcal/mol]        20.
MicroEnerStep[kcal/mol]       0.1
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*************************************************
!          MODEL SECTION
!*************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!
Model
!
 EnergyRelaxation                         ! Default collisional energy relaxation kernel
  Exponential                             ! Currently the only possible energy relaxation model
    Factor[1/cm]              400         ! (Delta_E_down)^(0) @ standard T (300 K)
    Power                     0.7         ! Power n in the expression (Delta_E_down) = (Delta_E_down)^(0)
(T/T0)^(n)
    ExponentCutoff            10          ! if (Delta_E) / (Delta_E_down) > value  transition probability is zero
  End
!
 CollisionFrequency                       ! Collision frequency model
  LennardJones                            ! Currently the only possible collisional frequency model  based on LJ
potential
    Epsilons[1/cm]            273.8  79.23        ! Epsilon_1 and Epsilon_2 (630.4 x kB x Na = 1.25)(cm-1 to K
= x 1.4) Ar and C5H5 (from Lindstedt et al )
```

```
      Sigmas[angstrom]                 5.78   3.47              ! Sigma_1 and Sigma_2 (from Lindstedt et al )
      Masses[amu]                      99      39.948           ! Masses of the buffer gas molecule and of the complex (check
order)
   End
!
!**********************************************
!***********************************
 Well RC
 Species
 RRHO     ! fake well
 Geometry[angstrom]            14
 C              0.46745900    0.33633100    1.17476800
 C              0.99260800   -0.86739500    0.87241800
 C              1.56145300   -0.81965400   -0.48516500
 C              1.37469100    0.40982400   -0.99468000
 H             -0.02202600    0.61671400    2.09672700
 H              1.01350400   -1.73481400    1.51948200
 H              2.04551000   -1.65177100   -0.97789000
 H              1.67764900    0.75420400   -1.97332400
 C              0.67249000    1.26821300    0.01621200
 H             -0.27341800    1.67771000   -0.35749400
 H              1.28820500    2.12818800    0.30701500
 O             -2.47871700    0.31790700    0.05443700
 O             -1.90795400   -0.68474200   -0.55626500
 H             -1.04825800   -0.81946700   -0.10122000
       Core        RigidRotor
            SymmetryFactor    1
       End
Frequencies[1/cm]          36
47.368204
58.391963
93.889598
110.080644
173.715166
344.905616
421.403793
516.19423
671.429829
722.087303
792.297067
796.353025
894.726157
909.773961
942.314551
950.704469
956.307771
```

```
986.919031
1079.202212
1097.775481
1100.289624
1234.373694
1236.983576
1284.656942
1357.698524
1375.131364
1438.868997
1530.348048
1607.025772
2965.443745
2997.773942
3130.563935
3142.551486
3159.409213
3165.184302
3441.815692
 ZeroEnergy[kcal/mol]           -5.9
 ElectronicLevels[1/cm]          1
    0.0                  2
End
End
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
!  REACTANTS
!***************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***************************************************
Bimolecular REACS
Fragment REACT1
RRHO
Geometry[angstrom]             11
C              0.00015600   -0.28081200    1.17594600
C              0.00015600    0.98779800    0.73475200
C              0.00015600    0.98779800   -0.73475200
C              0.00015600   -0.28081200   -1.17594600
H              0.00019600   -0.60649500    2.20697000
H              0.00032600    1.87799900    1.35003400
H              0.00032600    1.87799900   -1.35003400
H              0.00019600   -0.60649500   -2.20697000
C             -0.00053900   -1.21425500    0.00000000
H              0.87792900   -1.87097300    0.00000000
H             -0.87948000   -1.87034400    0.00000000
```

```
      Core        RigidRotor
            SymmetryFactor    2
      End
   Frequencies[1/cm]          27
332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
 0.000000000000000E+000   1.00000000000000
 End
 !***********************************
Fragment REACT2
 RRHO
 Geometry[angstrom]             3
 O              0.05494400   -0.59907100    0.00000000
 H             -0.87910200   -0.87306800    0.00000000
 O              0.05494400    0.70820400    0.00000000
      Core        RigidRotor
            SymmetryFactor    1
      End
   Frequencies[1/cm]          3
```

```
1218.783175
1416.714003
3596.0228
 ZeroEnergy[kcal/mol]             0.0
 ElectronicLevels[1/cm]                    1
 0.000000000000000E+000   2.00000000000000
End
GroundEnergy[kcal/mol] 0.0
End
!************************************************
!!!!  PRODUCTS             !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!************************************************
Bimolecular ProdS
Fragment Prod1
RRHO
Geometry[angstrom]              10
C              -0.00007800   -0.35099600    1.16853400
C              -0.00007800    0.94378900    0.73860100
C              -0.00007800    0.94378900   -0.73860100
C              -0.00007800   -0.35099600   -1.16853400
H               0.00038200   -0.69970600    2.18955800
H               0.00125900    1.83135400    1.35549300
H               0.00125900    1.83135400   -1.35549300
H               0.00038200   -0.69970600   -2.18955800
C              -0.00010300   -1.18505500    0.00000000
H              -0.00079100   -2.26648000    0.00000000
      Core        RigidRotor
           SymmetryFactor    10
      End
   Frequencies[1/cm]          24
328.999168
489.124246
508.641713
682.343299
725.107204
814.03079
819.329512
894.783969
907.829111
910.64279
934.474138
1035.7175
1050.867445
1120.71666
1193.86533
1255.526193
```

```
1355.146163
1475.063286
1511.608909
3127.261085
3143.895518
3152.533174
3164.305967
3172.474628
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
 0.000000000000000E+000   2.00000000000000
End
!***********************************
Fragment Prod2 !H2O2
 RRHO
 Geometry[angstrom]             4
 O              0.00000000    0.71225200   -0.05261700
 H              0.81812000    0.90119100    0.42093700
 O              0.00000000   -0.71225200   -0.05261700
 H             -0.81812000   -0.90119100    0.42093700
       Core        RigidRotor
            SymmetryFactor   2
       End
    Frequencies[1/cm]          6
420.136876
1005.234183
1297.911604
1445.39603
3746.028159
3746.69969
 ZeroEnergy[kcal/mol]            0.0
 ElectronicLevels[1/cm]                  1
    0.000000000000        1.00000000000000
End
GroundEnergy[kcal/mol] -4.2
End
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!***********************************
Barrier B1 REACS RC
RRHO
Stoichiometry  C5H7O1
Core  PhaseSpaceTheory
FragmentGeometry[angstrom]   11
C              0.00015600   -0.28081200    1.17594600
C              0.00015600    0.98779800    0.73475200
C              0.00015600    0.98779800   -0.73475200
```

C 0.00015600 -0.28081200 -1.17594600
H 0.00019600 -0.60649500 2.20697000
H 0.00032600 1.87799900 1.35003400
H 0.00032600 1.87799900 -1.35003400
H 0.00019600 -0.60649500 -2.20697000
C -0.00053900 -1.21425500 0.00000000
H 0.87792900 -1.87097300 0.00000000
H -0.87948000 -1.87034400 0.00000000
FragmentGeometry[angstrom] 3
O 0.05494400 -0.59907100 0.00000000
H -0.87910200 -0.87306800 0.00000000
O 0.05494400 0.70820400 0.00000000
SymmetryFactor 1
PotentialPrefactor[au] 154.4
PotentialPowerExponent 6
End
Frequencies[1/cm] 30
332.084544
509.421787
669.551133
713.253707
790.582689
791.932929
895.1354
912.984855
953.100466
956.303503
956.304958
992.348994
1079.532206
1098.603667
1104.302805
1238.59591
1287.731842
1360.894674
1378.870811
1535.110845
1613.176251
2964.034626
2996.215443
3123.541814
3129.63128
3145.081246
3153.91523
1218.783175
1416.714003

3596.0228
ZeroEnergy[kcal/mol] 0
ElectronicLevels[1/cm] 1
0.0000000000000000 2.0000000000000000
End
!**********
Barrier B2 RC ProdS
RRHO
Geometry[angstrom] 14
C -0.76605200 0.56735600 -1.12287900
C -1.27413700 -0.65361100 -0.83538900
C -1.32357600 -0.81386300 0.62430100
C -0.84372800 0.31213000 1.20676400
H -0.59976000 0.99312200 -2.10202900
H -1.61012300 -1.39326500 -1.54998000
H -1.68170800 -1.69625400 1.13636300
H -0.73007300 0.49705000 2.26452900
C -0.39182300 1.21574800 0.14921800
H 0.87510300 0.94105800 0.14696800
H -0.38659700 2.29574500 0.26724900
O 2.00726700 0.40090700 -0.02541200
O 1.77233100 -0.92608100 0.08840800
H 1.49226800 -1.20262400 -0.79915300
Core RigidRotor
SymmetryFactor 1
End
Rotor Hindered
Group 14
Axis 12 13
Symmetry 1
Potential[kcal/mol] 15
0
0.9405
3.67422
7.90647
12.77199
7.36725
3.27921
0.73359
0.01254
0.068
1.07844
3.65543
7.41741
3.65552
1.07848

End
Rotor Hindered
Group 13 14
Axis 10 12
Symmetry 1
Potential[kcal/mol] 15
0
0.084108915
0.258411153
0.568339761
0.959242284
1.072457166
1.135157166
1.166507166
1.153967166
1.172777166
1.222937166
1.216667166
0.956107284
0.642607284
0.102918915
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1782.087395
WellDepth[kcal/mol] 19
WellDepth[kcal/mol] 17.3
End

Frequencies[1/cm] 33
148.912945
225.144857
451.516667
458.715619
535.498879
637.959882
719.275079
726.836714
776.598975
808.591903
885.52658
909.386543
928.026548
932.833965
941.965157
978.888207
1006.699077

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1069.767701
1105.85335
1118.186803
1238.319363
1283.826331
1364.424116
1378.656247
1403.81019
1491.234932
1552.538641
3081.292591
3116.696427
3127.661986
3150.120396
3154.617995
3629.828173
  ZeroEnergy[kcal/mol]    13.1
  ElectronicLevels[1/cm]                    1
  0.0000000000000000         2.0000000000000000
End
!
!
!
!*****************************************************
!                END OF INPUT
!*****************************************************
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!

End
```

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