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MACCCR/AFOSR Fuel Research Review
Gaithersburg, September 8-10, 2008.

Detailed and Simplified Chemical Kinetics of Aviation Fuels and Surrogates.

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Outline of Talk

Topics

- Brief overview of our methodology and target compounds.
- Improved models for the oxidation of aromatics. Example: The chemistry of cyclopentadienyl.
- The extension to the oxidation of indene and naphthalene using a reaction class based approach with key channels identified via detailed path analysis and with rates determined using *ab initio* methods.
- The procurement of improved thermodynamic data for critical species: A systematic treatment.
- Future work

- :

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Brief Overview

- Toluene, 1-Methylnapthalene and Propylbenzene chemistry studied with performance assessed using JSR, PFR and shock tube data.
- Application of a reaction class based approach with key pathways identified and subjected to further study.
- Major reaction classes and new pathways identified.
- New reactions/rates evaluated and updates applied for the three fuels.
- The current reaction class based approach can be applied to other alkyl substituted aromatic fuels that form part of surrogate fuel blends.

Challenges (= Problems = Difficulties = Bad)

- A key problem that has affected aromatics chemistry, including toluene and related naphthalene and 1-methyl naphthalene work, has been identified as the oxidation and thermal decomposition of C_5-ring structures (e,g. Lindstedt, Maurice and Meyer, Proc. Roy. Soc. Chem. 2001; Lindstedt and Rizos, Proc. Combust. Inst., 2002…….)
- A further issue of key concern is related to accurate thermodynamic data for large hydrocarbons and their principal breakdown products: Group additivity methods do not work sufficiently well in many cases.
- Examples of work performed in order to resolve these issues are given.

(Re-) Evaluation of the Chemistry of the Cyclopentadienyl radical

- A detailed investigation of C_5H_5 decomposition was performed and 21 chemical reactions selected for further study.
- Potential Energy Surfaces (PES) were calculated at the G3B3 level using Gaussian03 and compared to previous work (e.g. Zhong and Bozzelli 1998 and Kern et al. 1998).
- Rate controlling steps identified.
- Using thermochemical data from the G3B3 computations, reaction rates were calculated with a RRKM/Master-Equation approach using ChemRate 1.5.2 (Tsang and Mokrushin) at 1 atm, 10 atm and the high pressure limit. We also evaluated **POLYRATE** (Truhlar and co-workers).
- ΔE_{down} collision values of 400 cm^{-1} where chosen to successfully model the pressure fall-off of reactions.
- The new reaction rates and thermochemical data have been test for a number of systems (not complete as yet – but close to).

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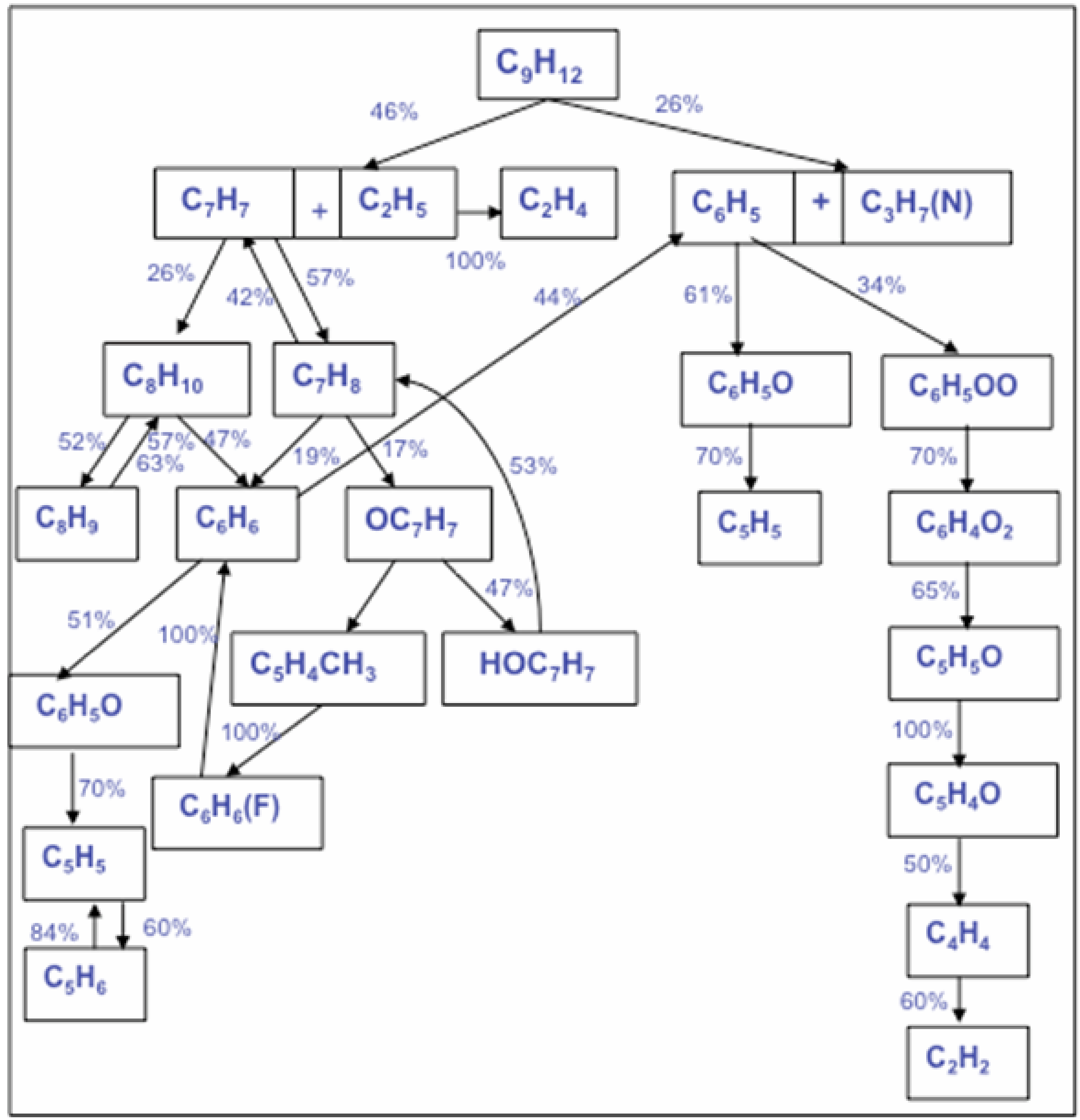
Why Cyclopentadienyl?

- The cyclopentadienyl radical forms a key part of the main reaction pathway leading from single ring aromatics to linear hydrocarbons. Comparatively few studies and significant uncertainties.
- The current study was performed as pre-cursor to an effort for indenyl using the same methodology.
- Example shown is from the oxidation of n-propyl benzene at 1100 K,1 atm pressure and a stoichiometry of 1.5.



Original Mechanism

Original C_5H_5 Mechanism : Rate Data for 21 reactions shown as parameters for the modified Arrhenius Equation

Reaction Number	Reactant 1	Reactant 2	Product 1	Product 2	A cm3 mol^{-1} s^{-1} / t-1	n	Ea kJ
1	C5H5	O2	C5H5O	O	7.73E+15	1.8	203.93
2	C5H5	O2	C5H5OO		7.31E+07	0.08	-40.04
3	C5H5	HO2	C5H4O	H2O	1.19E+33	-6.52	56.07
4	C5H5	HO2	C5H5O	OH	6.27E+29	-4.69	48.74
5	C5H5	O	C4H5(T)	CO	1.00E+14	0	0
6	C5H5	O	C5H4O	H	5.81E+13	-0.02	0.08
7	C5H5	O	C5H5O		1.00E+13	0	0
8	C5H5	OH	C5H4OH	H	3.00E+13	0	0
9	C5H5	OH	C5H5OH		6.49E+14	-0.85	-11.42
10	C5H5	OH	C5H5O	H	1.36E+51	-10.46	238.91
11	C5H5	OH	C4H6(T)	CO	4.00E+14	0	18.84
12	C5H5O		C4H5(T)	CO	7.50E+11	0	183.68
13	C5H5O		C5H4O	H	2.00E+14	0	78.16
14	C5H4OH		C5H4O	H	2.10E+13	0	200.83
15	C5H5OH		C5H4OH	H	6.00E+14	0	326.1
16	C5H5OH		C5H5O	H	1.09E+16	0	433.71
17	C5H5OO		C5H4O	OH	3.61E+12	0	156.06
18	C5H5OO		C5H5O	O	2.36E+14	0	245.68
19	C5H5		C3H3	C2H2	6.31E+13	-0.08	260.66
20	C5H5		C5H5(L)		3.90E+11	1.00	322.58
21	C5H5(L)		C3H3	C2H2	3.70E+11	0.00	124.70

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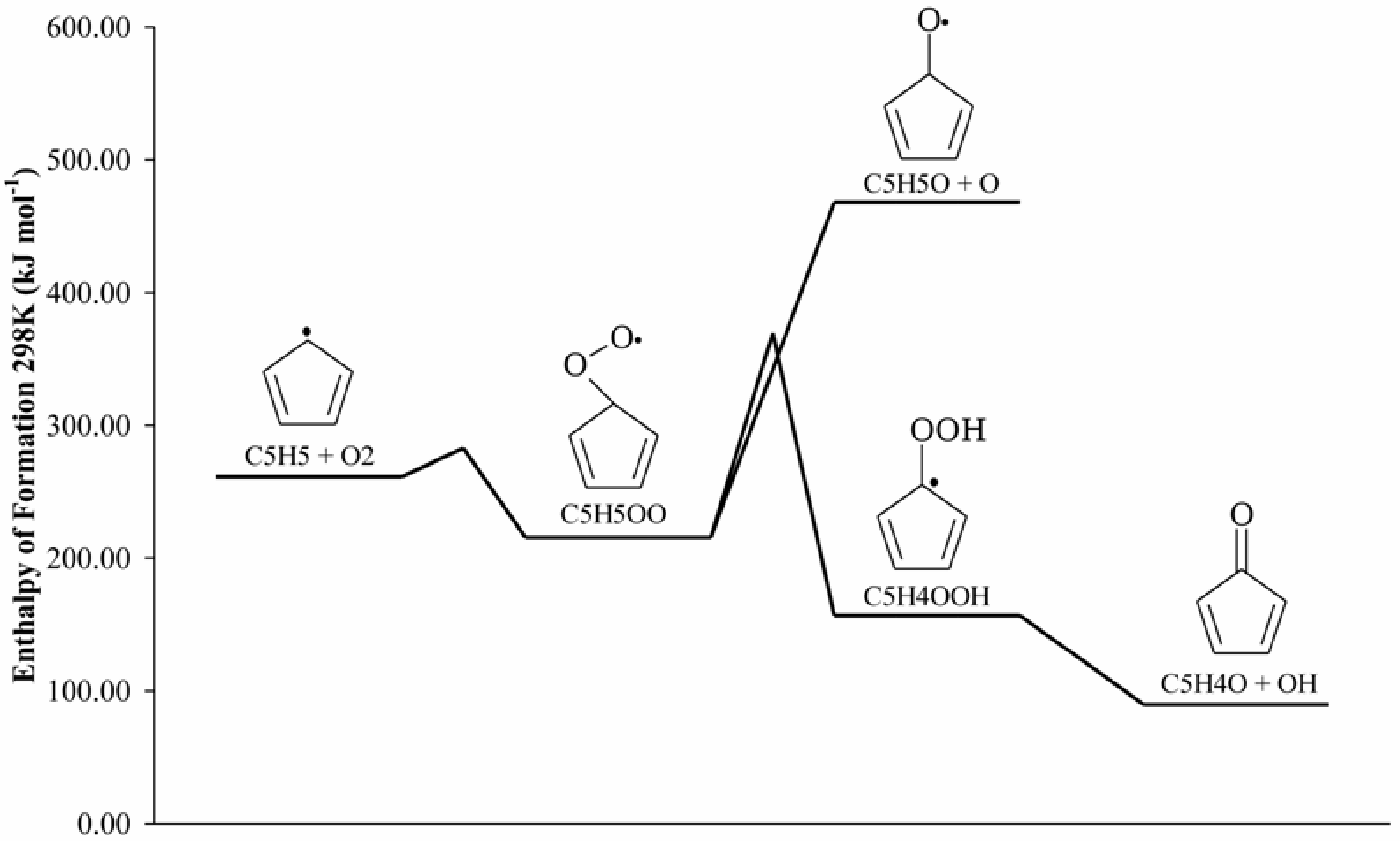
Potential energy for $C_5H_5+O_2$ reactions



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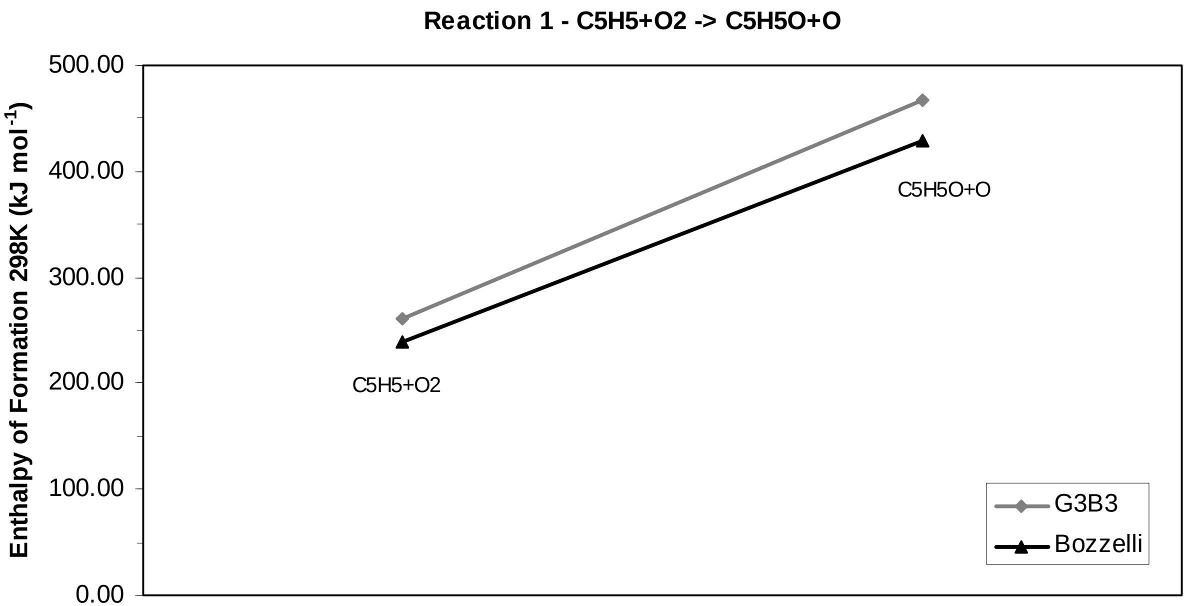
Reaction 1 – $C_5H_5 + O_2 \rightarrow C_5H_5O + O$



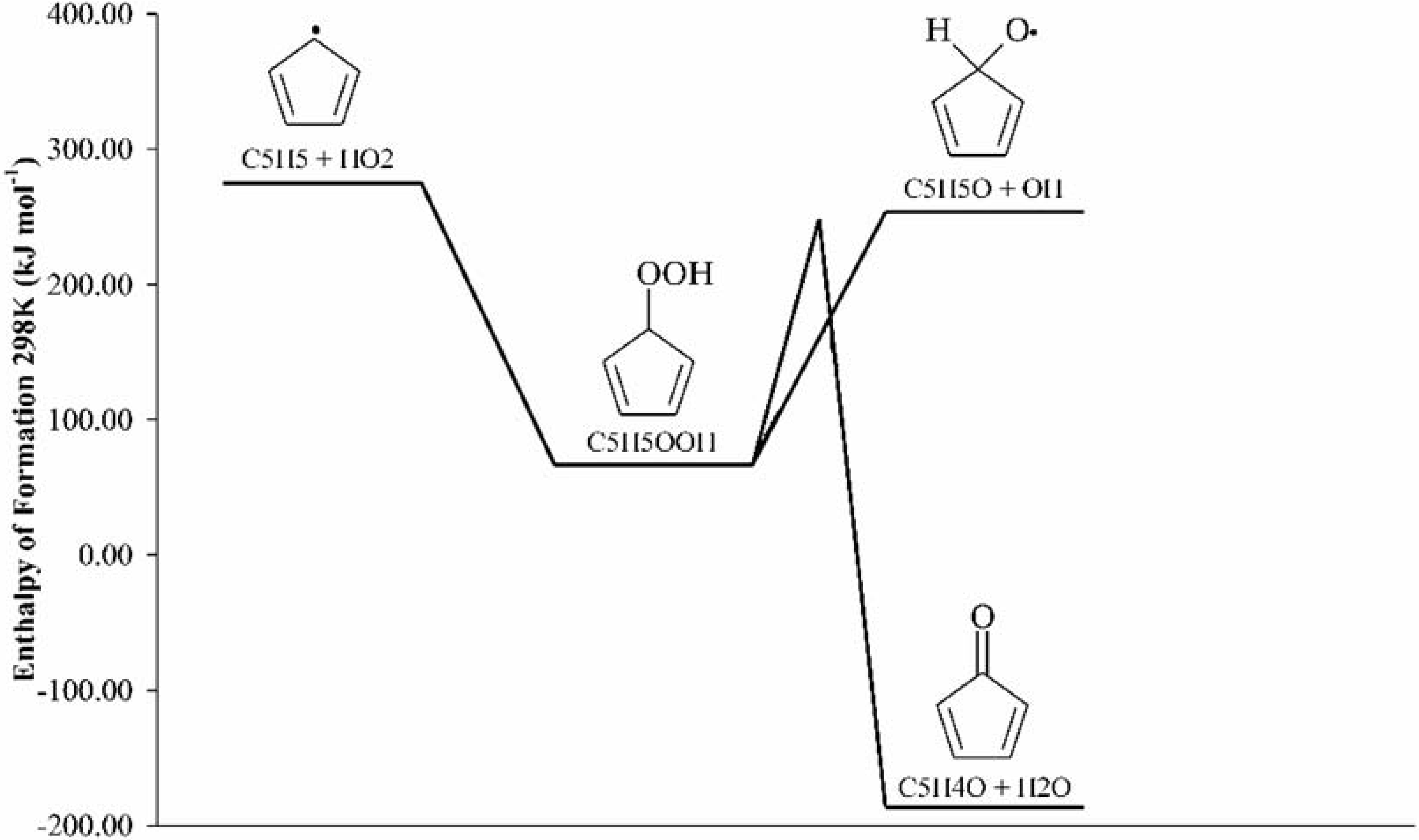
	Bozzelli[1]	pw
	HP	HP
A ($cm^3\ mol^{-1}\ s^{-1}$)	7.73E+15	9.52E+04
n	-0.73	1.80
Ea (kJ)	203.93	218.53

T	k	K
500	4.1E-08	1.0E-13
600	1.3E-04	9.1E-10
700	3.9E-02	6.3E-07
800	2.8E+00	8.7E-05
900	7.9E+01	4.2E-03
1000	1.1E+03	9.3E-02
1200	5.8E+04	1.0E+01
1400	9.6E+05	3.1E+02
1600	7.8E+06	4.1E+03
1800	3.9E+07	3.2E+04
2000	1.4E+08	1.7E+05

- The reaction is a bimolecular transfer of the oxygen atom with no immediate steps.
- The G3B3 PES showed a 17 kJ difference in the energy change as compared to the previous study.

1. Zhong and Bozzelli, J. Phys. Chem. A, 1998, 102, 3537

Potential Energy for C_5H_5+HO_2 reactions



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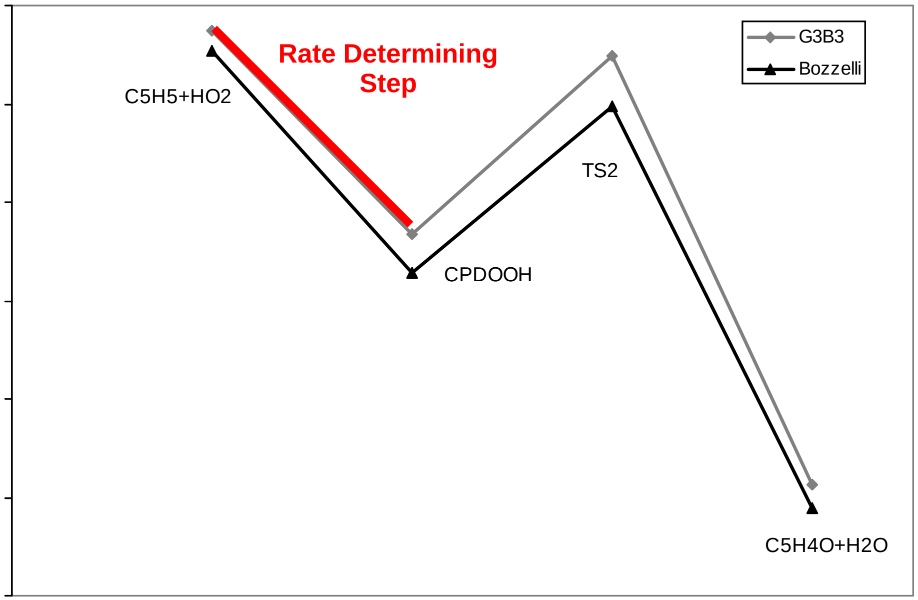
Reaction 3 – $C_5H_5 + HO_2 \rightarrow C_5H_4O + H_2O$



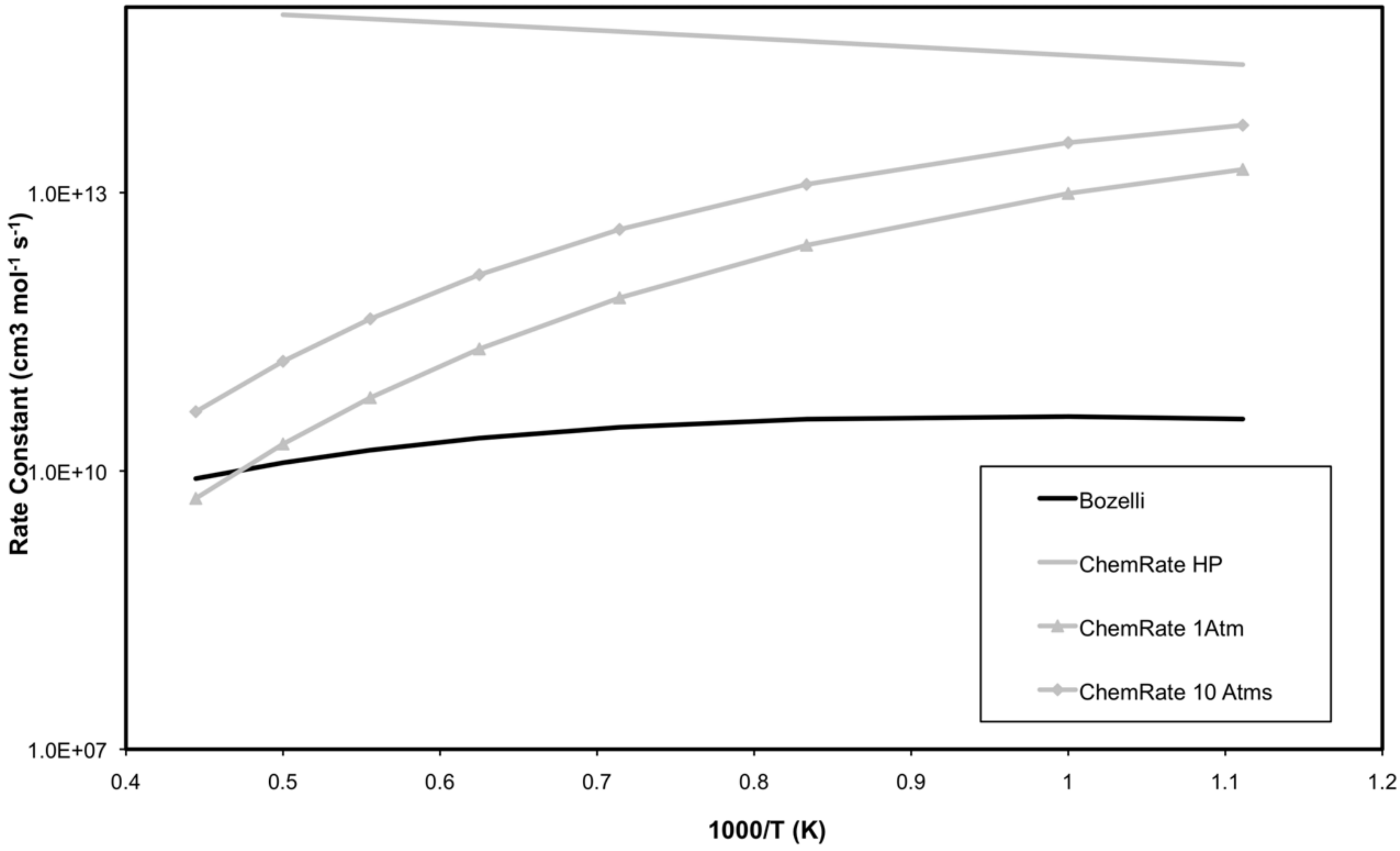
	Bozzelli[1]	pw	pw	pw
	1 Atm	1 Atm	10 Atm	HP
A($cm^3\ mol^{-1}\ s^{-1}$)	1.19E+33	6.25E+65	1.13E+66	1.56E+16
n	-6.52	-16.16	-15.89	-0.23
Ea (kJ)	56.07	82.83	92.87	19.37

T	k	k	k	k
500	4.2E+09	3.4E+13	3.0E+13	3.5E+13
600	1.2E+10	4.9E+13	6.8E+13	7.2E+13
700	2.2E+10	4.4E+13	8.3E+13	1.2E+14
800	3.1E+10	3.0E+13	7.3E+13	1.8E+14
900	3.6E+10	1.8E+13	5.3E+13	2.4E+14
1000	3.9E+10	9.8E+12	3.5E+13	3.0E+14
1200	3.6E+10	2.7E+12	1.2E+13	4.3E+14
1400	3.0E+10	7.4E+11	4.0E+12	5.5E+14
1600	2.3E+10	2.1E+11	1.3E+12	6.5E+14
1800	1.7E+10	6.2E+10	4.4E+11	7.5E+14
2000	1.2E+10	2.0E+10	1.5E+11	8.3E+14

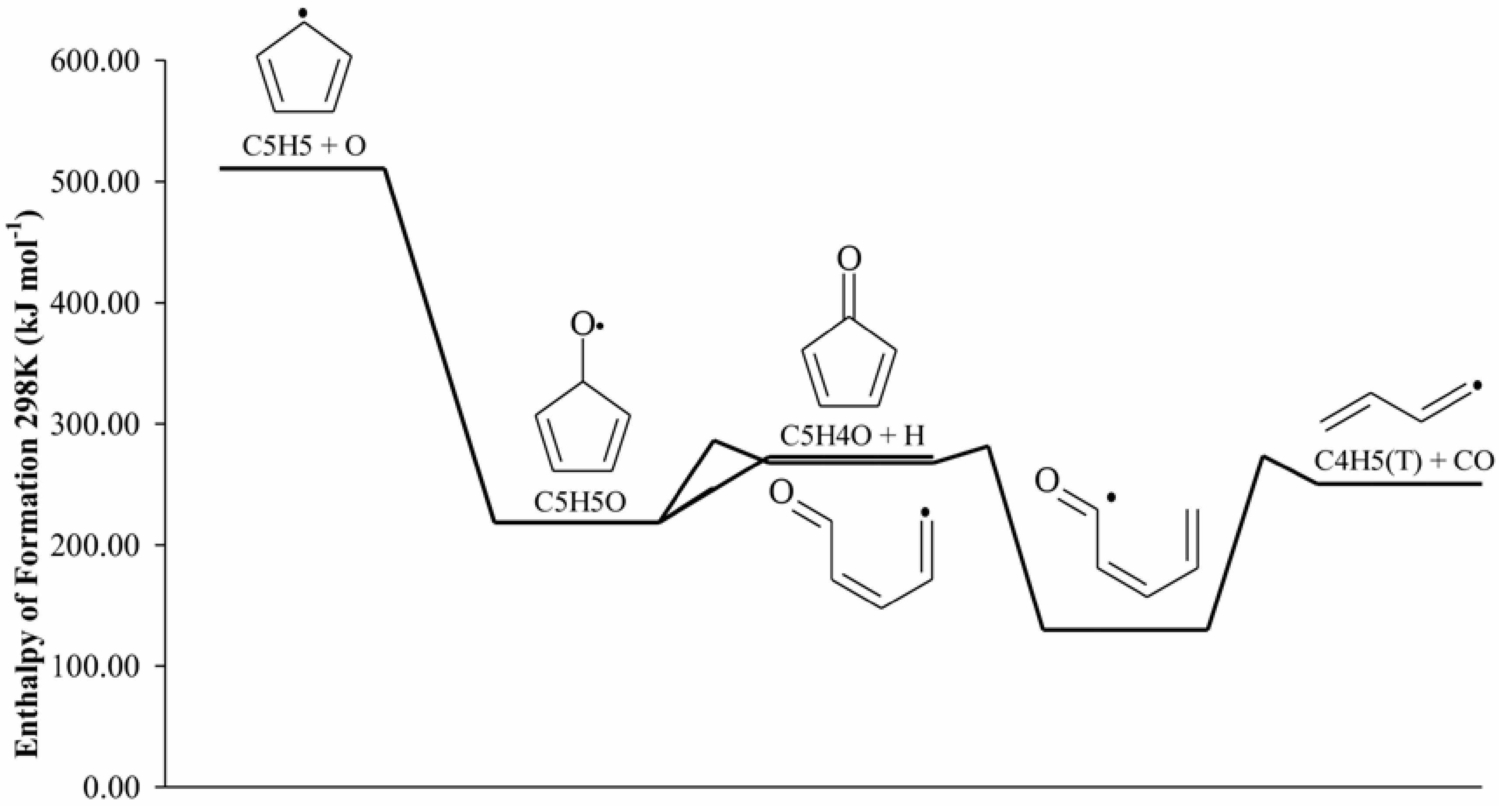
- The PES at the G3B3 level showed reasonable fit to previous studies.
- As in previous studies it was assumed that CPDOOH will not stabilise, leading to the first step controlling the overall reaction rate.

1. Zhong and Bozzelli, J. Phys. Chem. A, 1998, 102, 3537.

Reaction 3 – $C_5H_5 + HO_2 \rightarrow C_5H_4O + H_2O$



Potential energy for C_5H_5+O reactions



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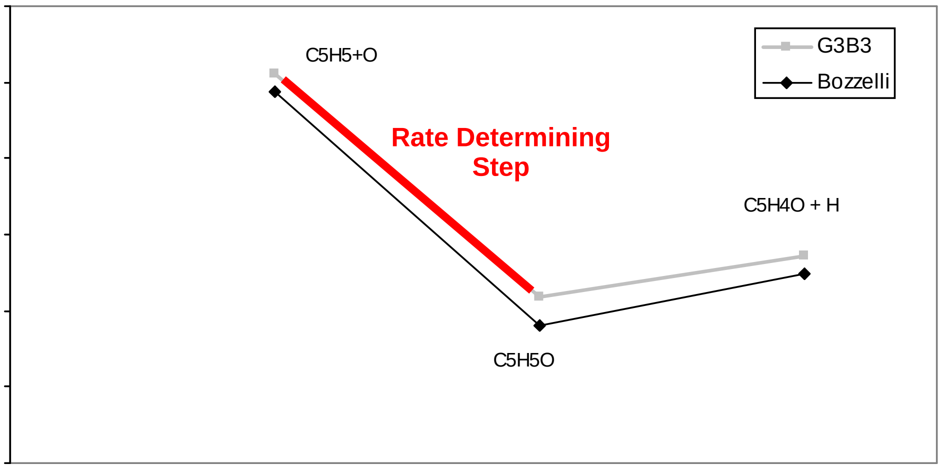
Reaction 6 – $C_5H_5 + O \rightarrow C_5H_4O + H$



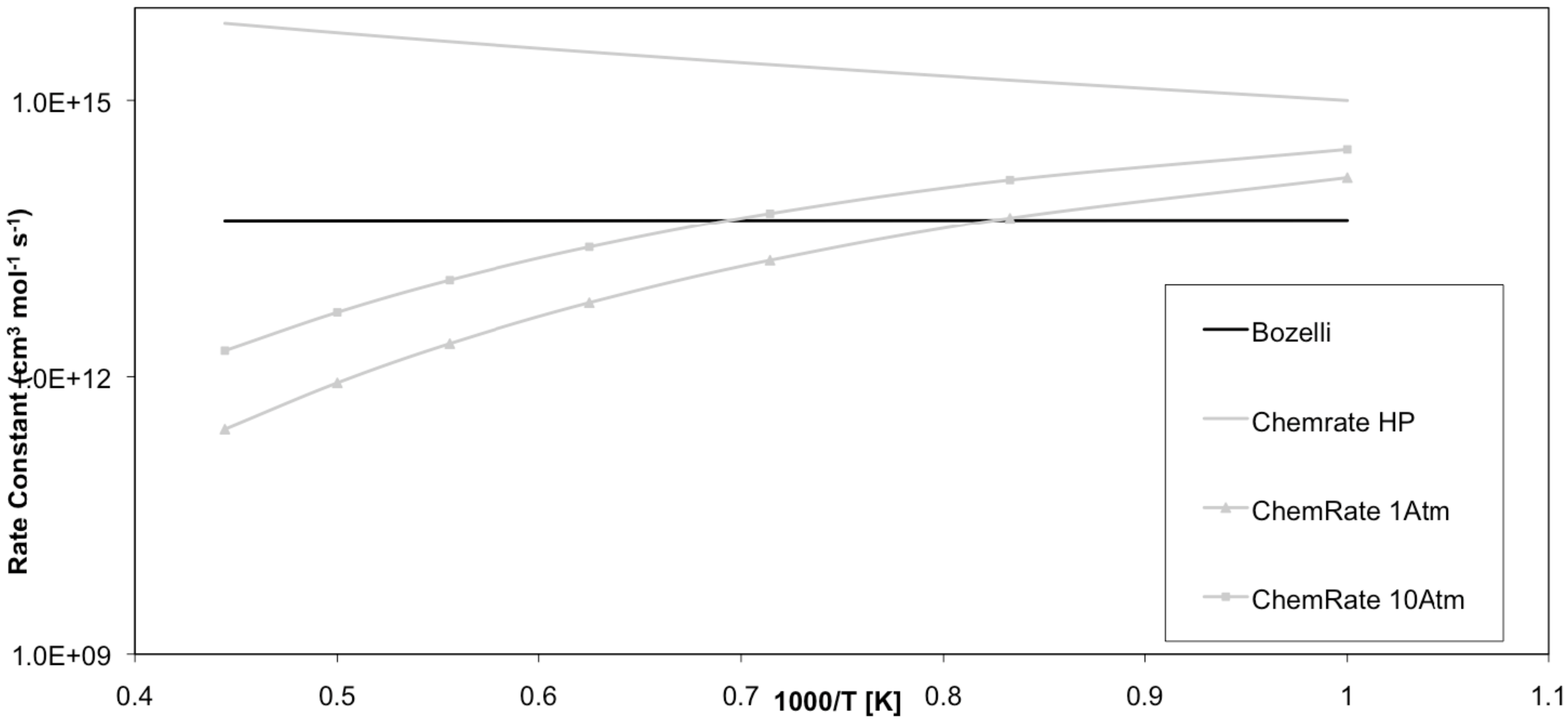
	Bozzelli[1]	pw	pw	pw
		1 Atm	10 Atm	HP
A($cm^3\ mol^{-1}\ s^{-1}$)	5.81E+13	1.54E+61	1.22E+55	1.82E+12
n	-0.02	-14.29	-12.26	1.17
Ea (kJ)	0.08	79.33	73.40	14.59

T	k	k	k	k
500	5.0E+13	2.1E+14	2.1E+14	7.7E+13
600	5.0E+13	3.7E+14	4.3E+14	1.7E+14
700	5.0E+13	4.0E+14	5.3E+14	3.1E+14
800	5.0E+13	3.3E+14	5.0E+14	4.9E+14
900	5.0E+13	2.3E+14	4.0E+14	7.2E+14
1000	5.0E+13	1.5E+14	2.9E+14	1.0E+15
1200	5.0E+13	5.3E+13	1.4E+14	1.7E+15
1400	5.0E+13	1.8E+13	5.9E+13	2.4E+15
1600	5.0E+13	6.3E+12	2.5E+13	3.3E+15
1800	5.0E+13	2.3E+12	1.1E+13	4.3E+15
2000	5.0E+13	8.6E+11	5.0E+12	5.4E+15

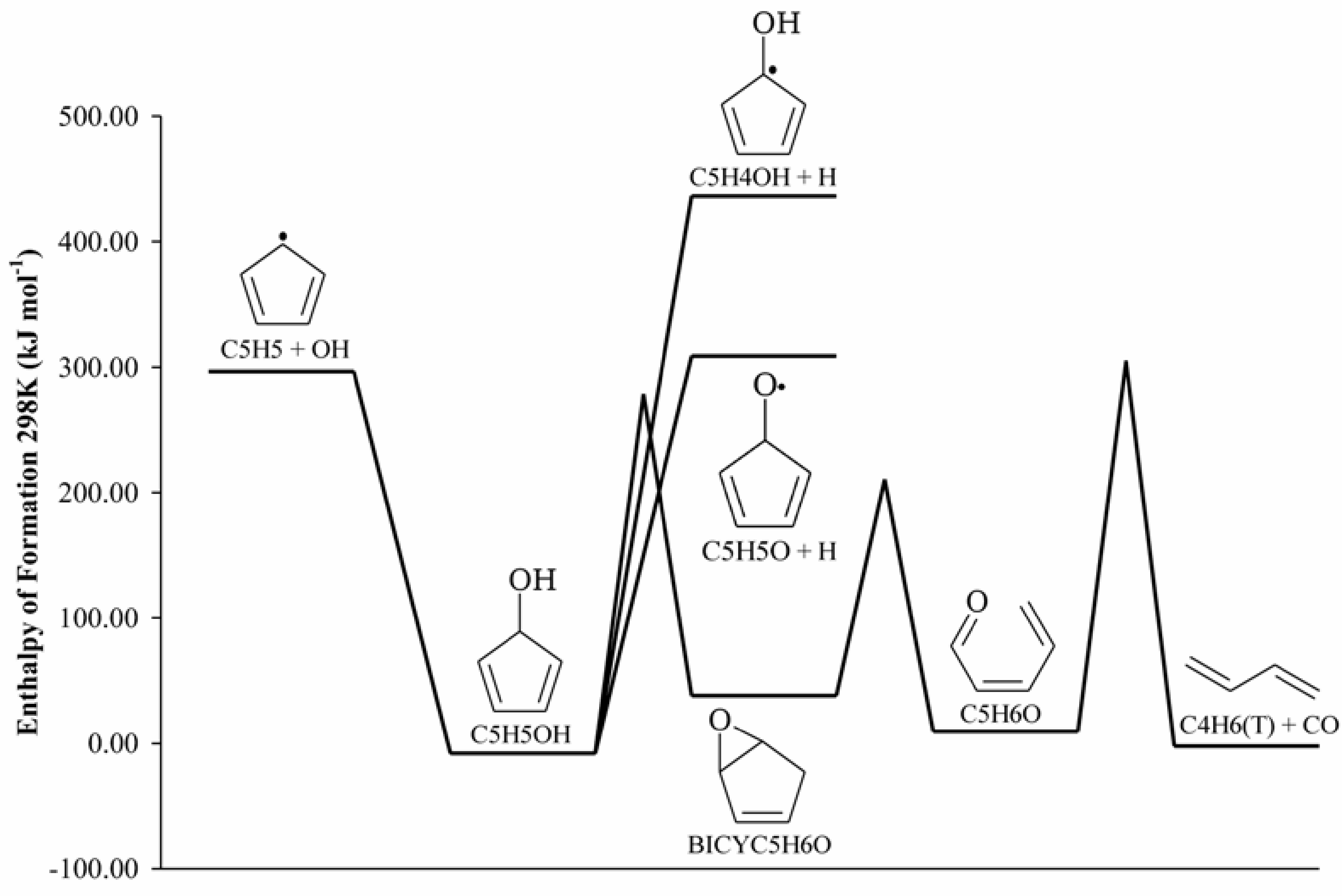
- The PES at the G3B3 level showed reasonable fit the previous study.
- Again the first step was assumed to be rate controlling as the energy barrier for the second step was small and it was assumed the reaction would not stabilise at the intermediate.

1. Zhong and Bozzelli, J. Phys. Chem. A, 1998, 102, 3537

Reaction 6 – $C_5H_5 + O \rightarrow C_5H_4O + H$



Potential energy for C_5H_5+OH reactions



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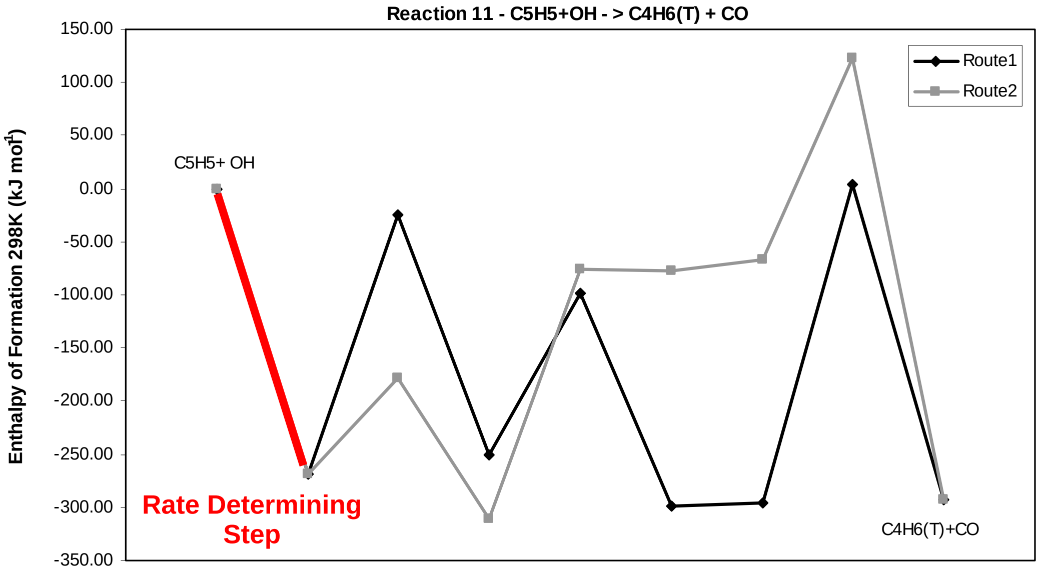
Reaction 11 – C_5H_5+ OH → C_4H_6(T) + CO

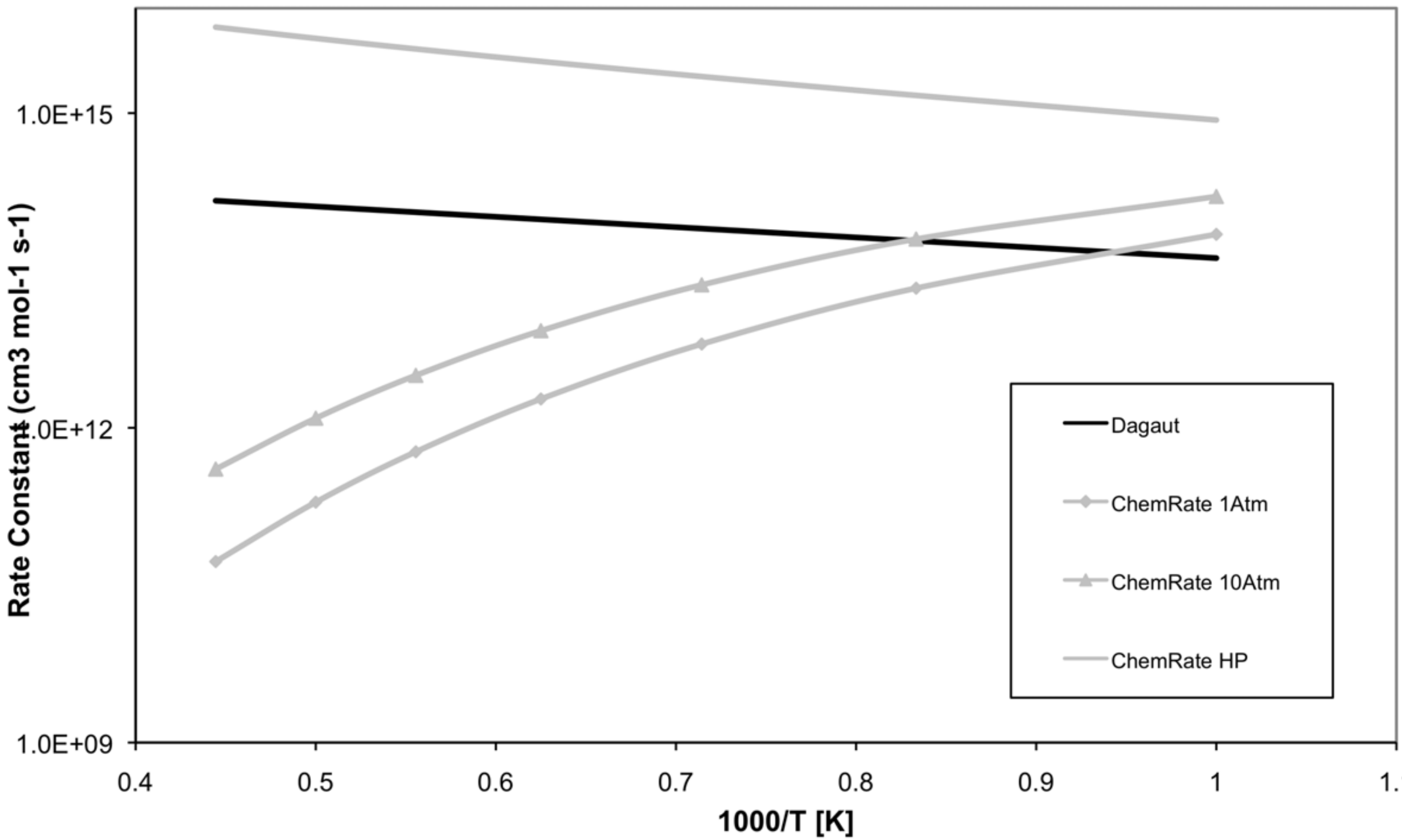


- No previous in depth study of the potential energy surface of this reaction.
- Two routes were explored for the breakdown of the C_5H_5 ring.
- Route 1 proceeded along a lower energy path and, as none of steps have a higher energy than the reactants, rates were calculated for the first step.

	Dagaut & Ristori	pw	pw	pw
	1 Atm	1 Atm	10 Atm	HP
A(cm3 mol^{-1} s^{-1})	4.00E+14	1.59E+66	6.41E+60	1.94E+12
n	0.00	-15.95	-14.11	1.17
Ea (kJ)	18.84	86.11	81.71	16.35

T	k	k	k	k
500	4.3E+12	1.4E+14	1.5E+14	5.4E+13
600	9.2E+12	2.4E+14	3.1E+14	1.3E+14
700	1.6E+13	2.4E+14	3.6E+14	2.4E+14
800	2.4E+13	1.8E+14	3.2E+14	4.1E+14
900	3.2E+13	1.2E+14	2.4E+14	6.1E+14
1000	4.1E+13	7.0E+13	1.6E+14	8.6E+14
1200	6.1E+13	2.1E+13	6.3E+13	1.5E+15
1400	7.9E+13	6.3E+12	2.3E+13	2.2E+15
1600	9.7E+13	1.9E+12	8.4E+12	3.1E+15
1800	1.1E+14	5.9E+11	3.2E+12	4.1E+15
2000	1.3E+14	2.0E+11	1.2E+12	5.2E+15

Reaction 11 – $C_5H_5 + OH \rightarrow C_4H_6(T) + CO$



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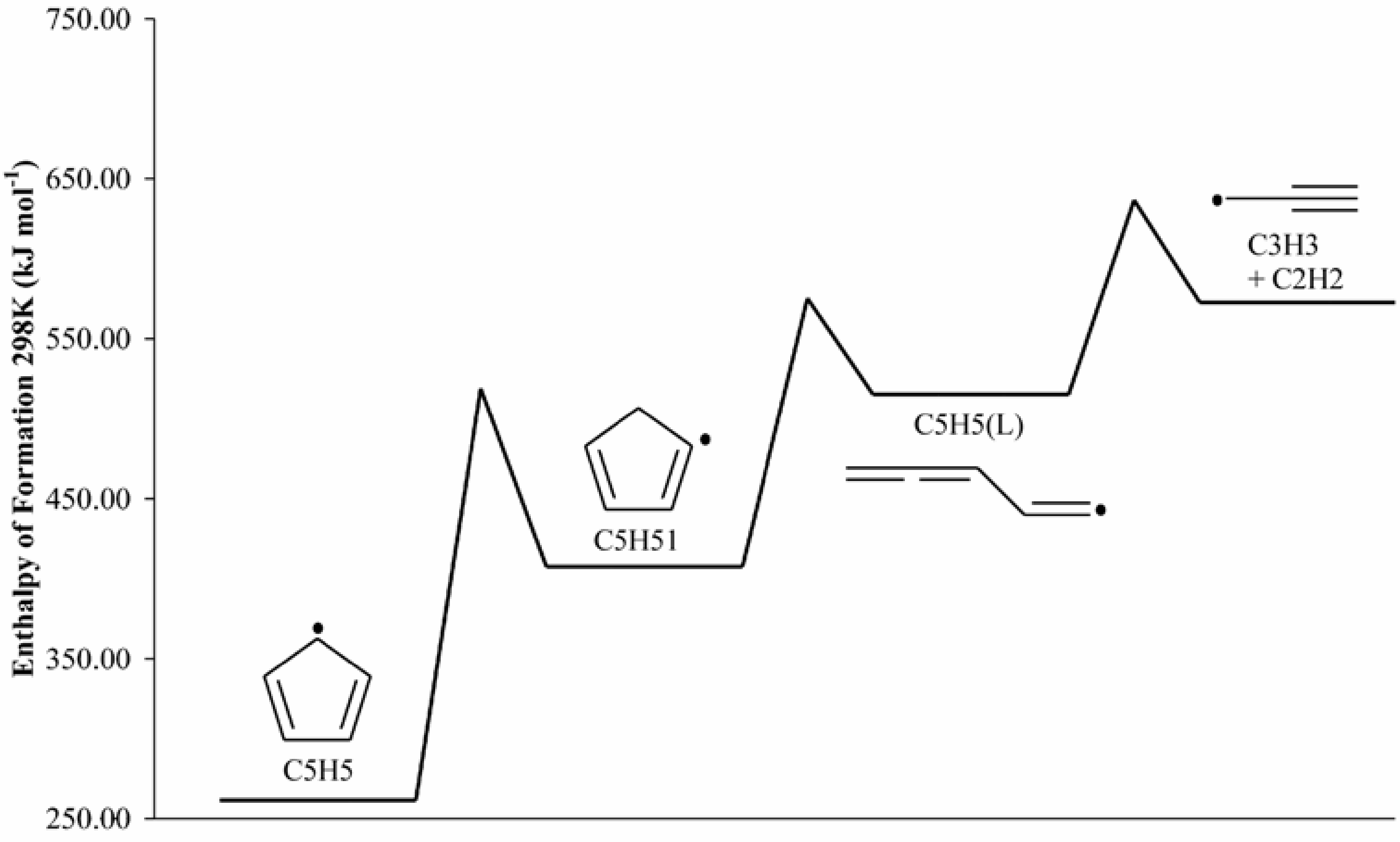
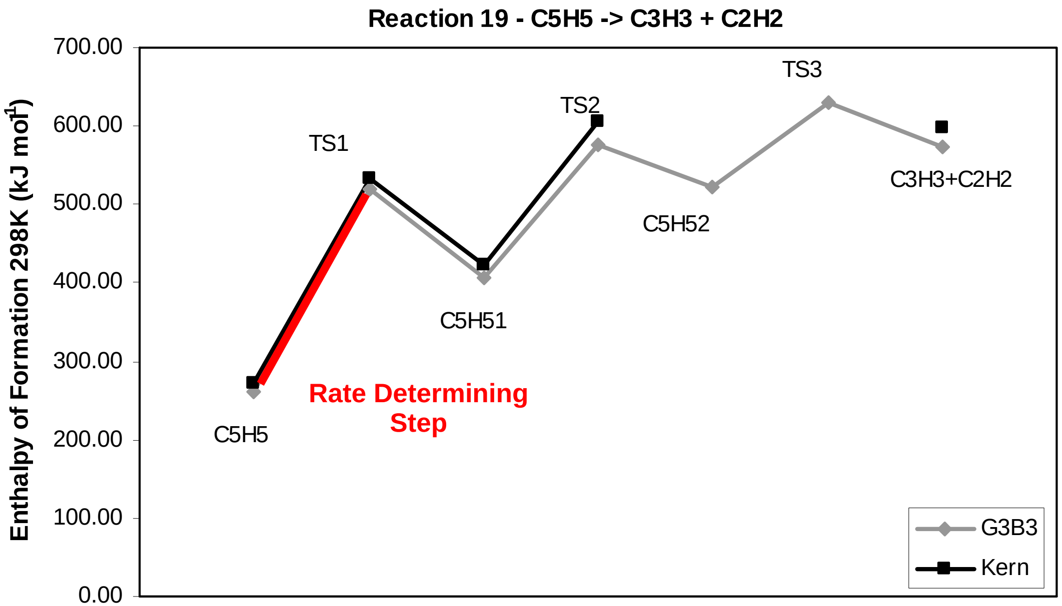
Potential energy for C_5H_5 thermal decomposition



Reaction 19 – $C_5H_5 \rightarrow C_3H_3 + C_2H_2$



	Kern[2]	pw	pw	pw
		1 Atm	10 Atm	HP
A($cm^3\ mol^{-1}\ s^{-1}$)	6.31E+13	1.074E+38	3.890E+27	4.654E+12
n	-0.08	-7.479	-4.328	0.114
Ea (kJ)	260.66	307.552	288.472	259.073

T	k	k	k	k
500	2.2E-14	5.2E-15	5.9E-15	8.1E-15
600	7.7E-10	3.0E-10	2.8E-10	2.7E-10
700	1.3E-06	6.3E-07	5.6E-07	4.6E-07
800	3.5E-04	1.7E-04	1.6E-04	1.2E-04
900	2.7E-02	1.2E-02	1.2E-02	9.3E-03
1000	8.8E-01	3.4E-01	3.5E-01	3.0E-01
1200	1.6E+02	4.1E+01	5.1E+01	5.5E+01
1400	6.6E+03	1.1E+03	1.6E+03	2.3E+03
1600	1.1E+05	1.1E+04	2.0E+04	3.8E+04
1800	9.4E+05	5.8E+04	1.4E+05	3.3E+05
2000	5.3E+06	2.0E+05	5.9E+05	1.9E+06

- The previous study by Kern et al. (1998) used high level density functional theory to calculate enthalpies and shows a good fit to G3B3 theory.
- The first step has the highest energy barrier of 263 kJ and therefore controls the rate of this reaction channel. Similar rates in both studies.

2. R.D. Kern et al., Proc. Combust. Inst. 27, 1998 143.

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Updated C_5H_5 Mechanism

Reaction Number	Reactant 1	Reactant 2	Product 1	Product 2	A $cm^3\ mol^{-1}\ s^{-1} / s^{-1}$	n	Ea kJ
1	C5H5	O2	CYPD1O	O	9.518E+04	1.802	218.534
2	C5H5	O2	C5H5OO		2.258E+12	-1.519	5.077
3	C5H5	HO2	C5H4O	H2O	6.248E+65	-16.159	82.827
4	C5H5	HO2	CYPD1O	OH	6.248E+65	-16.159	82.827
5	C5H5	O	C4H5(T)	CO	2.126E+56	-12.566	89.965
6	C5H5	O	C5H4O	H	2.126E+56	-12.566	89.965
7	C5H5	O	CYPD1O		2.126E+56	-12.566	89.965
8	C5H5	OH	C5H4OH	H	2.237E+63	-14.757	102.021
9	C5H5	OH	CYPD1OH		2.237E+63	-14.757	102.021
10	C5H5	OH	CYPD1O	H	3.316E+63	-14.263	385.544
11	C5H5	OH	C4H6(T)	CO	2.237E+63	-14.757	102.021
12	CYPD1O		C4H5(T)	CO	1.752E+42	-8.769	267.356
13	CYPD1O		C5H4O	H	1.752E+42	-8.769	267.356
14	C5H4OH		C5H4O	H	2.288E+63	-15.097	245.372
15	CYPD1OH		C5H4OH	H	4.725E+56	-12.198	402.900
16	CYPD1OH		CYPD1O	H	3.319E+63	-14.263	385.545
17	C5H5OO		C5H4O	OH	1.320E+51	-11.538	221.574
18	C5H5OO		CYPD1O	O	6.694E+61	-14.023	344.670
19	C5H5		C3H3	C2H2	1.074E+38	-7.479	307.552
20	C5H5		C5H5(L)		1.074E+38	-7.479	307.552
21	C5H5(L)		C3H3	C2H2	3.314E+42	-9.463	148.237

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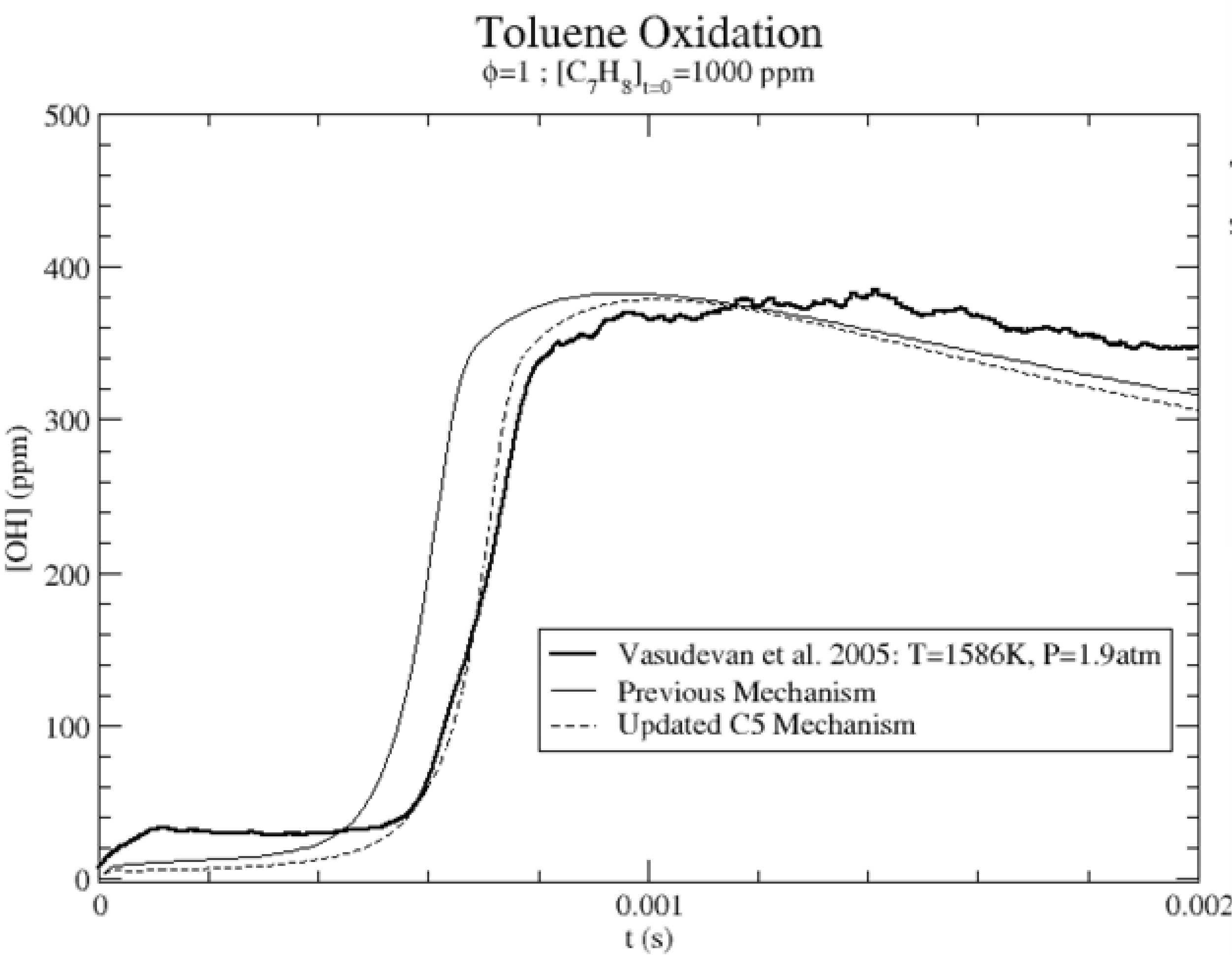
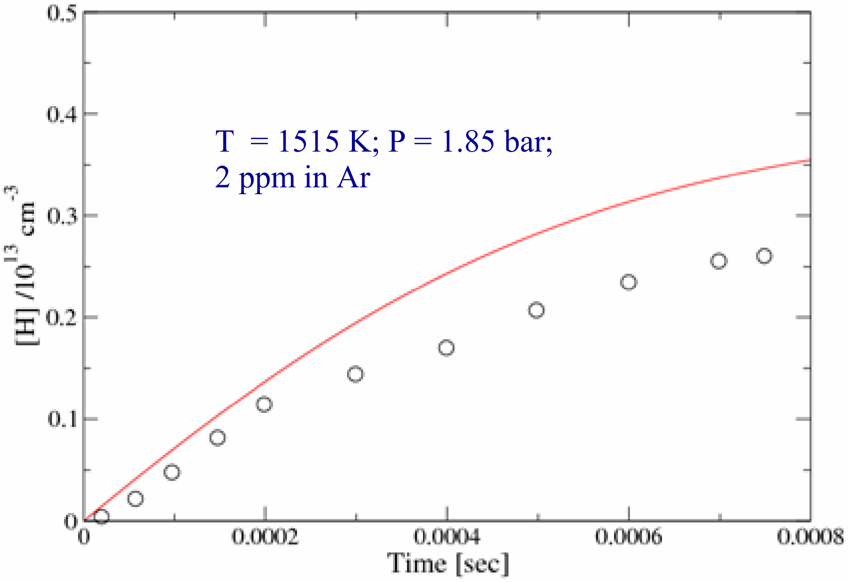
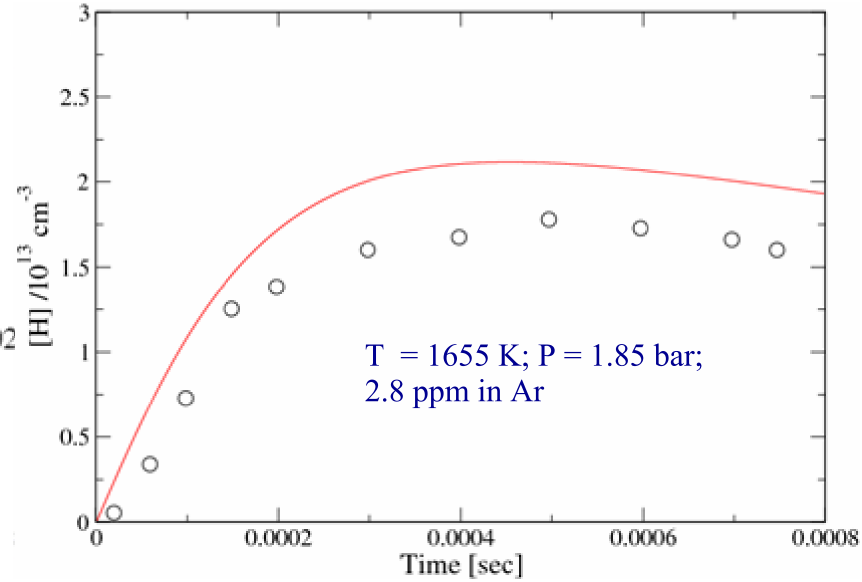
Sample Result: Toluene Oxidation







H radical measurements from Braun-Unkhoff et al. (1988)

OH radical measurements for Vasudevan et al. (2005).

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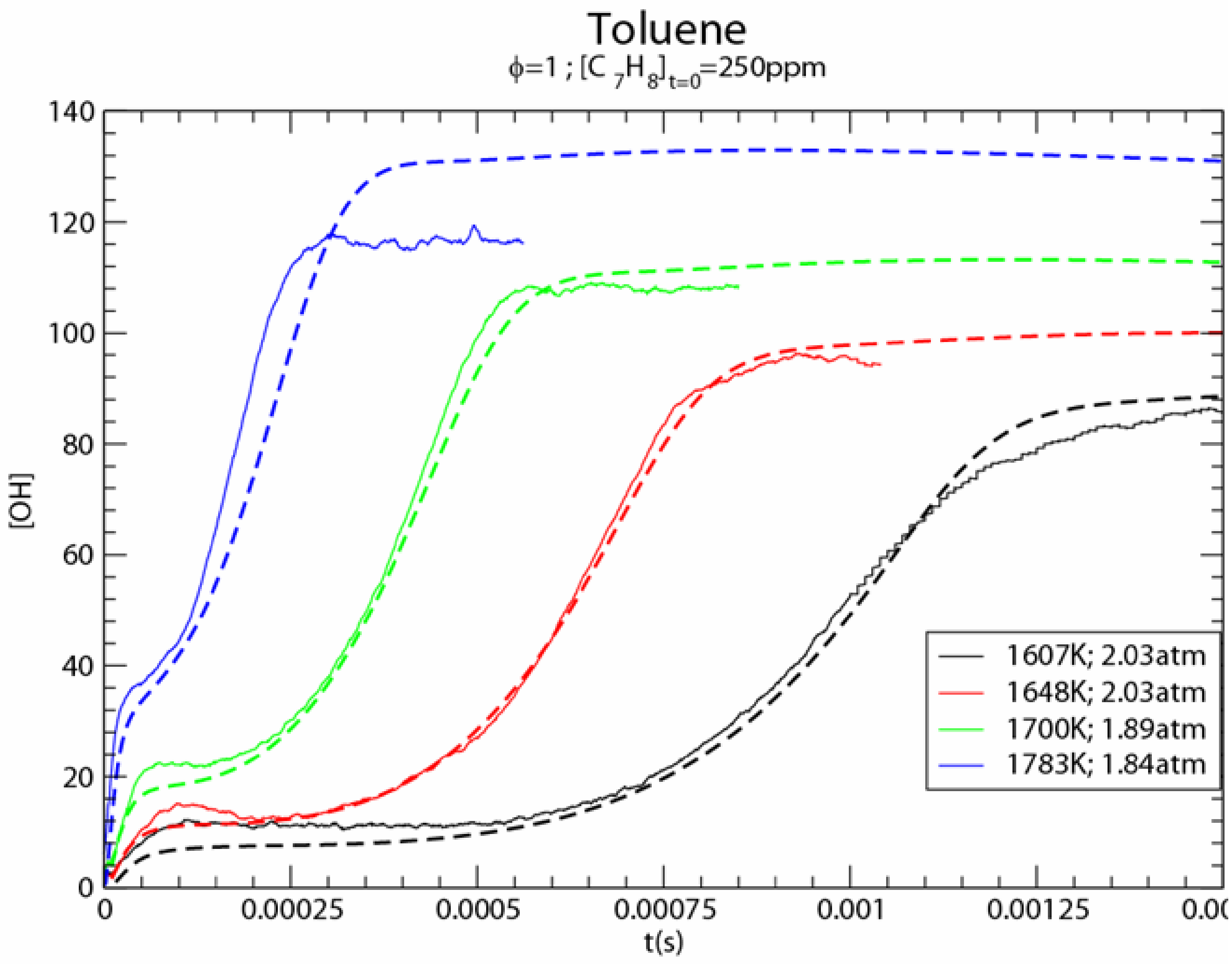
Sample Result: Toluene Oxidation

Examples of computations of the time resolved OH radical profile are compared with experimental data obtained by Hanson and co-workers

Solid line:
Experimental data

Dashed line:
Computations



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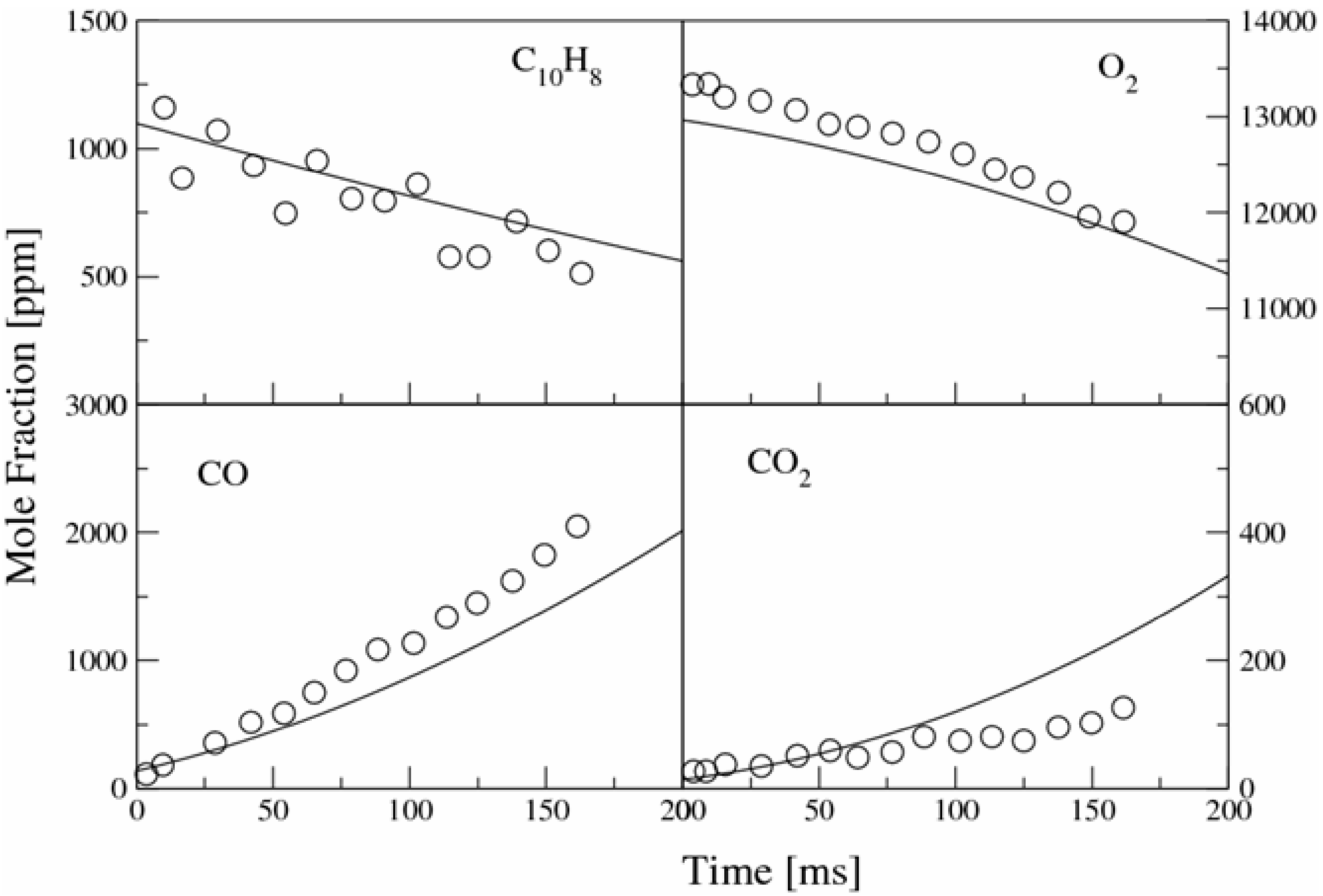
Sample Results: Naphthalene Oxidation

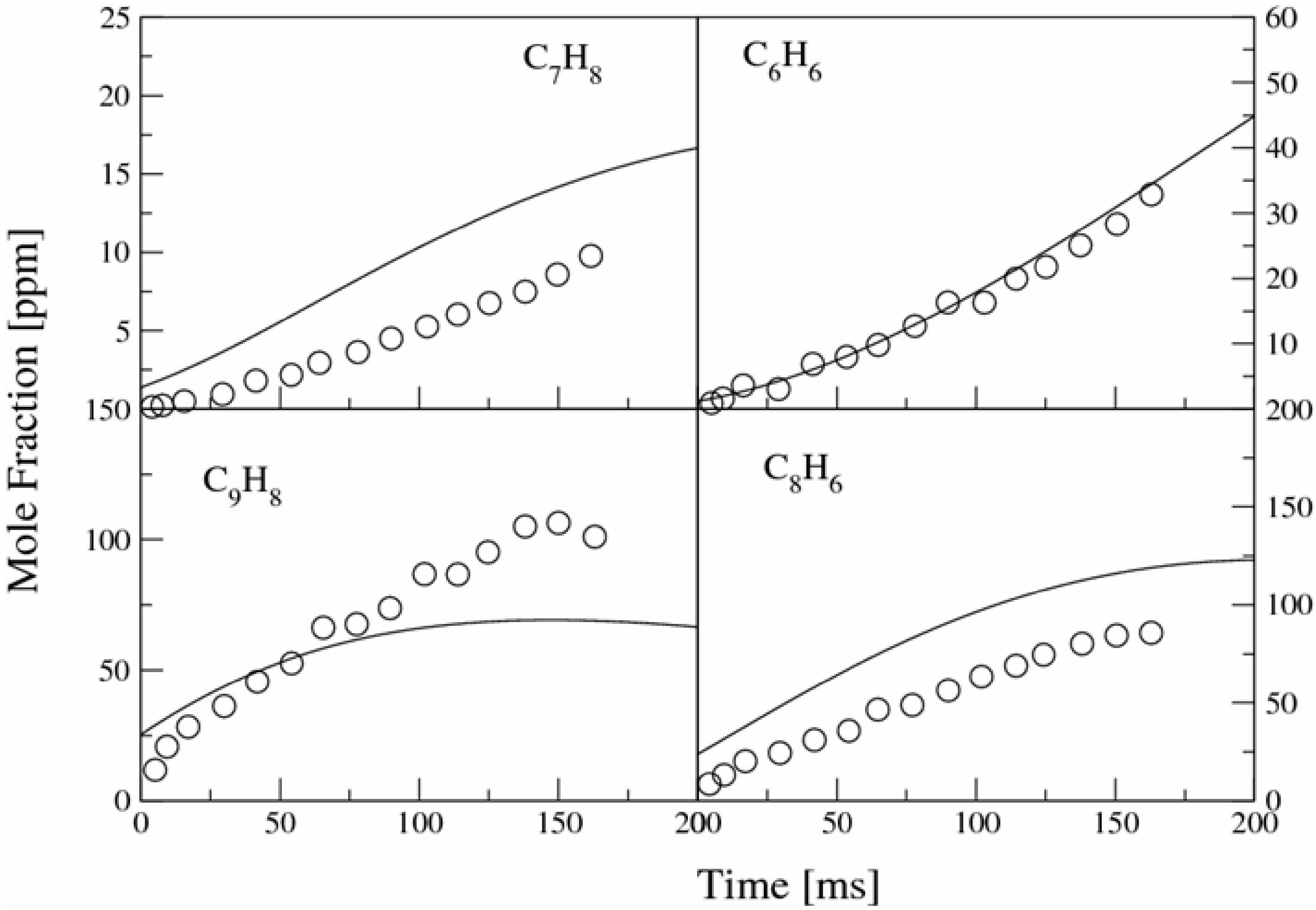
Concentration profiles of major species during naphthalene oxidation in the Princeton plug flow reactor for a stoichiometry of Φ = 1.1, temperature 1197 K using updated C_5H_5 and C_9H_7 mechanisms.



□Experimental data from Shaddix and coworkers (1993). Computations from Lindstedt, Markaki and Robinson, Proceedings of Anacapri workshop on Fine Carbon Based Particles (2008).

Naphthalene Oxidation

Major intermediate aromatics



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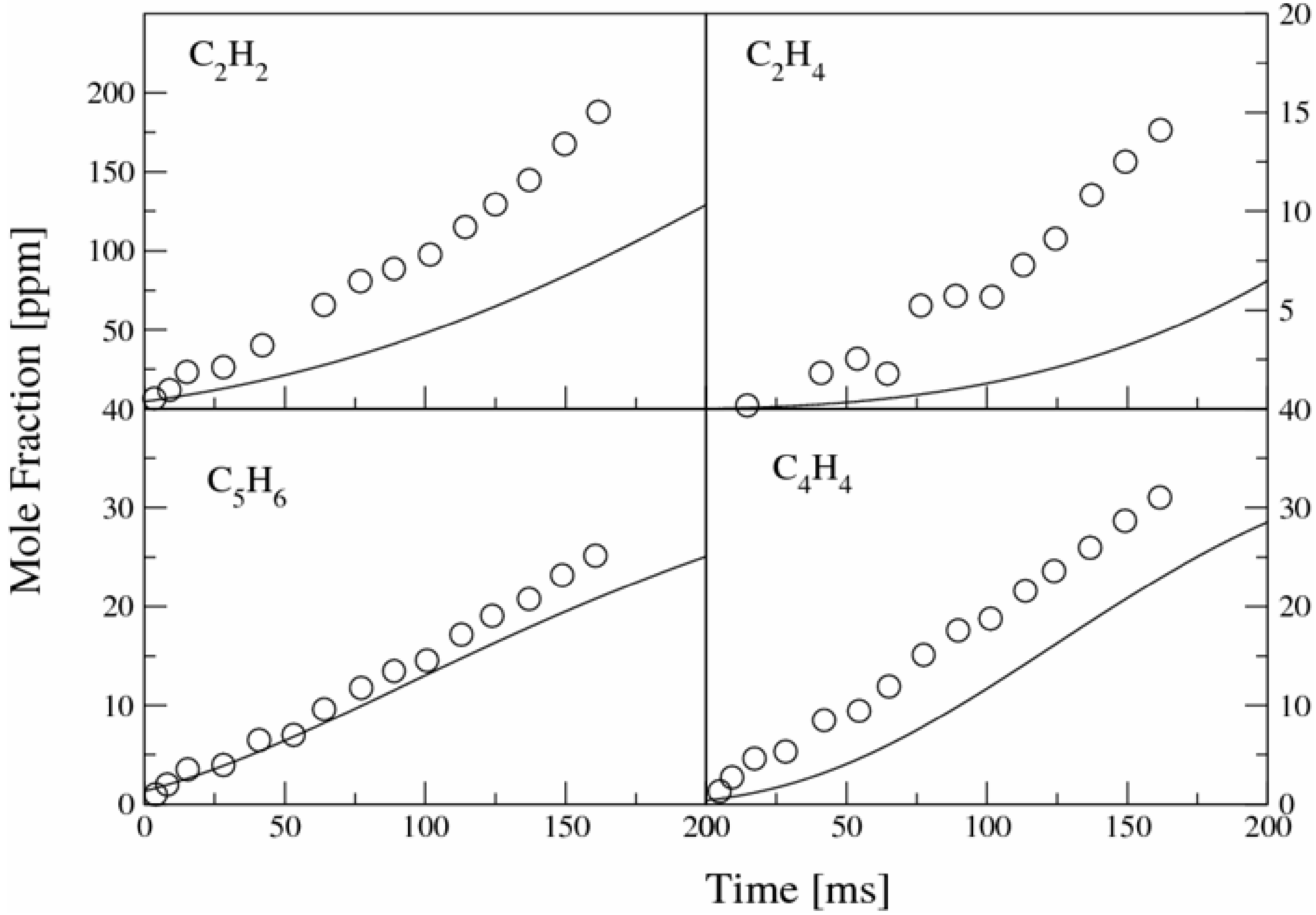
Naphthalene Oxidation

Major products



Thermodynamic Database

- Thermodynamic data was calculated in the temperature range 200 - 6000 K. DFT and G3B3/G3MP2B3 composite quantum mechanical methods were using to supply data for statistical mechanics calculations.
- JANAF Polynomials have been produced for a wide range of C_5-C_{10} species with an updated C_1 – C_4 database having been reconciled with Wang (USC).
- The process now has high degree of automation allowing calculation for larger species including accurate contributions from internal rotation rather than estimates which are often used.
- Access to a high performance cluster with 64 CPU's now allows accurate thermochemical calculations of long chain hydrocarbons such as decane and its derivatives.

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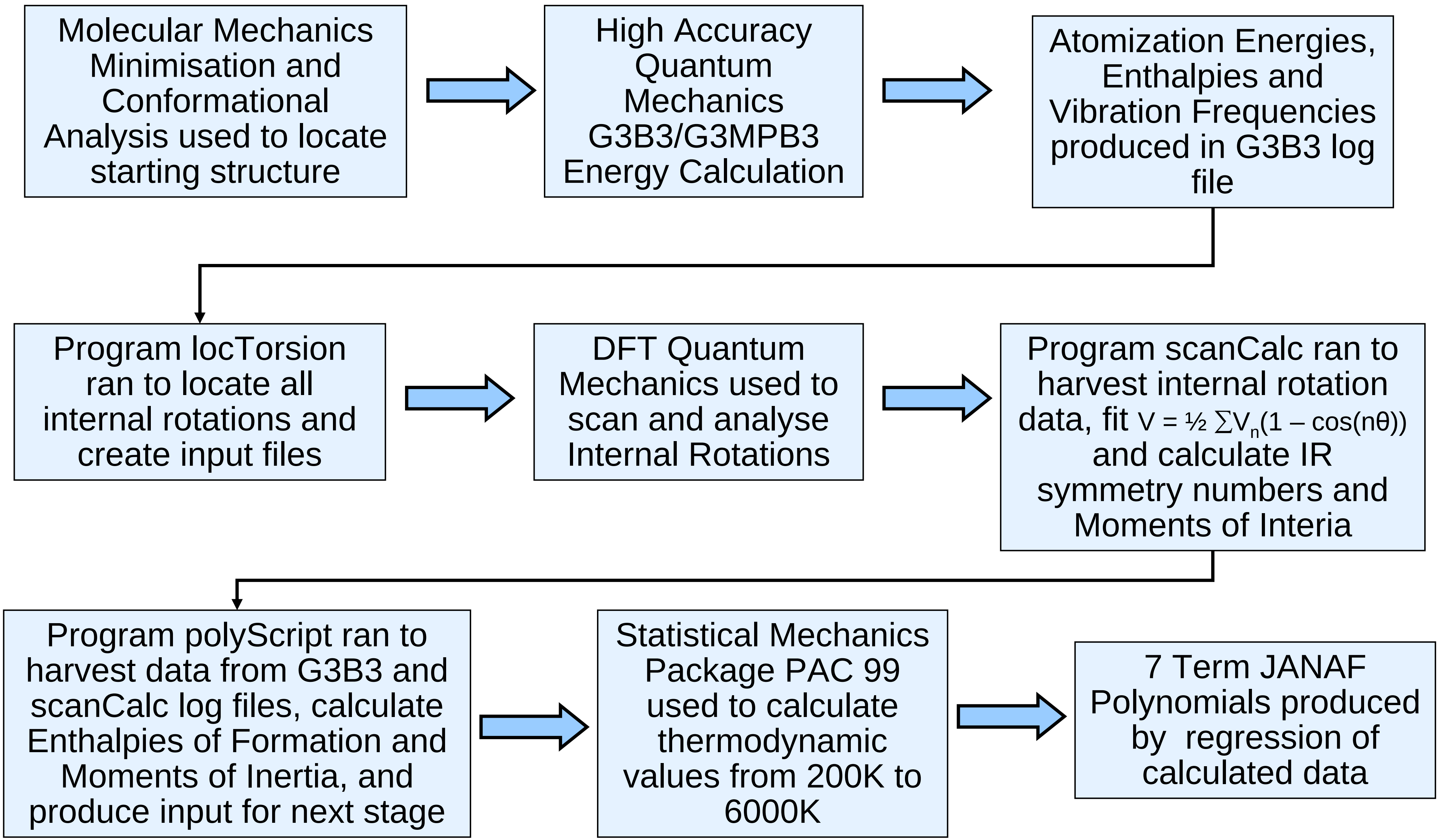
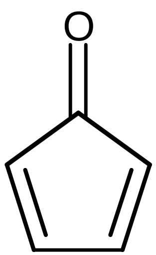
Semi-Automated Thermodynamic Method



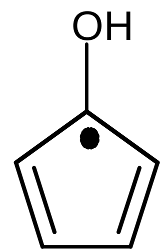
Example Species and updated G3B3 Thermodynamic Data

C5H4O



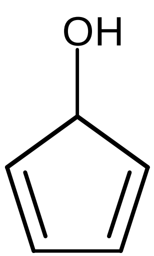
Calculated Data	
$\Delta_f H_{298}$	54.750
S_{298}	291.420
C_{p298}	84.202
$\Delta_f H_{1000}$	156.309

C5H4OH



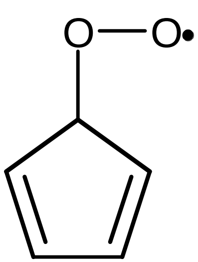
Calculated Data	
$\Delta_f H_{298}$	90.831
S_{298}	309.168
C_{p298}	95.931
$\Delta_f H_{1000}$	204.583

C5H5OH



Calculated Data	
$\Delta_f H_{298}$	-8.135
S_{298}	309.393
C_{p298}	100.137
$\Delta_f H_{1000}$	112.777

C5H5OO



Calculated Data	
$\Delta_f H_{298}$	215.590
S_{298}	352.445
C_{p298}	105.554
$\Delta_f H_{1000}$	338.507

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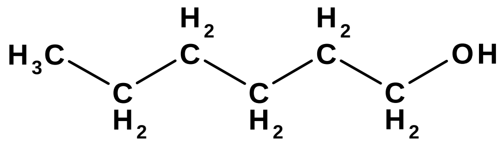
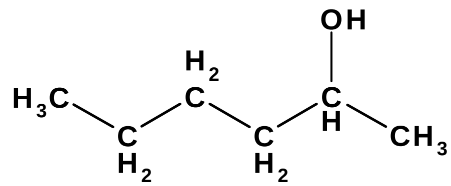
Thermodynamic Database

Thermodynamic data was produced for C_7 based species such as heptanol, derivates and radicals.

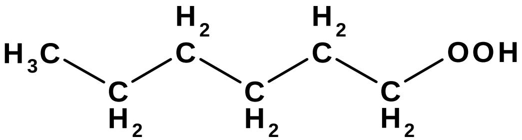
1-Heptanol
$\Delta_f H_{298}$=-339.25 kJ/mol



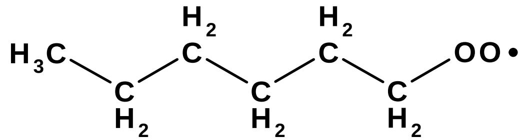
2-Heptanol
$\Delta_f H_{298}$=-357.49 kJ/mol



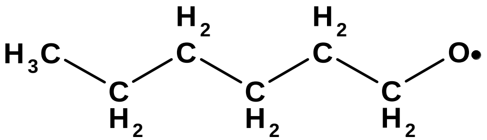
Heptane-1-hydroperoxide
$\Delta_f H_{298}$=-266.60 kJ/mol



Heptane-1-peroxide
$\Delta_f H_{298}$=-127.50 kJ/mol



Heptanal Radical
$\Delta_f H_{298}$=-122.24 kJ/mol



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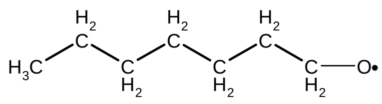
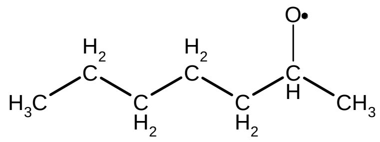
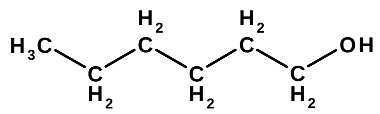
Thermodynamic Database

Example: Section from thermodynamic database

Name	Acronym	Structure	Mol. Weight	ΔfH298 kJ/mol	Error ±kJ/mol	S298 J/mol/K	Cp298 J/mol/K	ΔfH1000 kJ/mol	Reference
Heptanal Radical	C7H15O		115.193	-122.234	± 8.00	509.348	189.77	90.838	Present Work
Heptan-2-al Radical	C7H15O-S		115.193	-132.441	± 8.00	507.527	189.679	81.13	Present Work
1-Heptanol	C7H15OH		116.201	-339.208	± 8.00	518.697	193.879	-121.082	Present Work

Example: JANAF polynomials from thermodynamic database

```
 C7H15O                            200K-6000K REF : G3B3    R.ROBINSON 01-Mar-07
  2.01723482E+01  3.83626958E-02 -1.40842882E-05  2.30214773E-09 -1.38884947E-13
 -2.42808401E+04 -6.88971586E+01  1.67580517E+01 -1.83086886E-02  1.90996861E-04
 -2.32436911E-07  8.96047054E-11 -2.01551879E+04 -3.53707686E+01
C7H15O-S                          200K-6000K REF : G3MP2B3 R.ROBINSON 05-Mar-07
  2.03872119E+01  3.81412590E-02 -1.40608687E-05  2.30204980E-09 -1.38972097E-13
 -2.55603316E+04 -7.02828342E+01  1.53821566E+01 -9.90059100E-03  1.74429270E-04
 -2.18709059E-07  8.54289033E-11 -2.12251954E+04 -2.96339556E+01
C7H15OH                           200K-6000K REF : G3B3    R.ROBINSON 01-Mar-07
  2.04179069E+01  3.94701269E-02 -1.43138803E-05  2.32349758E-09 -1.39572027E-13
 -5.04982176E+04 -6.94990031E+01  1.76511593E+01 -2.33129856E-02  2.08741927E-04
 -2.53164593E-07  9.78425705E-11 -4.64162556E+04 -3.84646181E+01
```

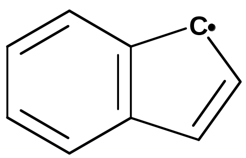
Sample G3B3 enthalpies of formation at 298 K compared to Thergas (Benson additivity method)

Species	G3B3 $\Delta_f H_{298}$ kJ/mol	Thergas $\Delta_f H_{298}$ kJ/mol	Imperial Thergas Residual
C7H13	145.06	141.33	3.72
1-C7H14	-63.28	-62.86	-0.42
2-C7H14	-73.07	-74.41	1.34
3-C7H14	-72.02	-74.73	2.71
1-C7H15	18.59	15.89	2.70
2-C7H15	7.09	6.68	0.40
3-C7H15	8.09	6.68	1.40
4-C7H15	8.09	6.68	1.40
C7H16	-188.23	-188.08	-0.15

Thermodynamic Database

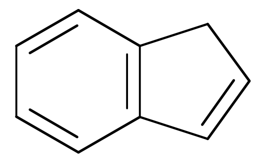
Further example species.

C9H7



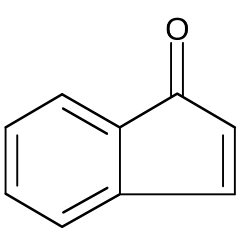
Calculated Data	
$\Delta_f H_{298}$	281.382
S_{298}	339.165
C_{p298}	123.666
$\Delta_f H_{1000}$	442.948

C9H8



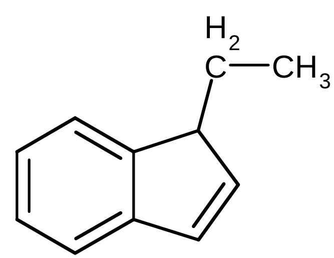
Calculated Data	
$\Delta_f H_{298}$	160.966
S_{298}	336.397
C_{p298}	125.242
$\Delta_f H_{1000}$	328.408

C9H6O



Calculated Data	
$\Delta_f H_{298}$	54.972
S_{298}	352.130
C_{p298}	132.103
$\Delta_f H_{1000}$	220.639

C9H12



Calculated Data	
$\Delta_f H_{298}$	7.737
S_{298}	408.342
C_{p298}	154.771
$\Delta_f H_{1000}$	204.994

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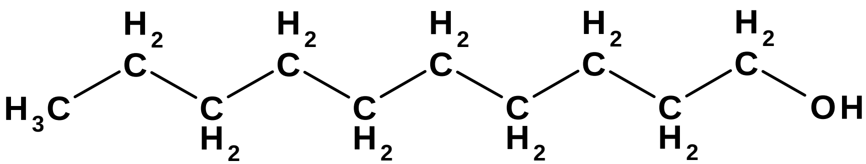
Thermodynamic Database

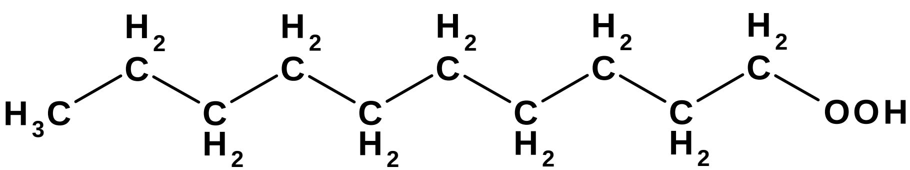
Example Species and Thermodynamic Data

Decanol



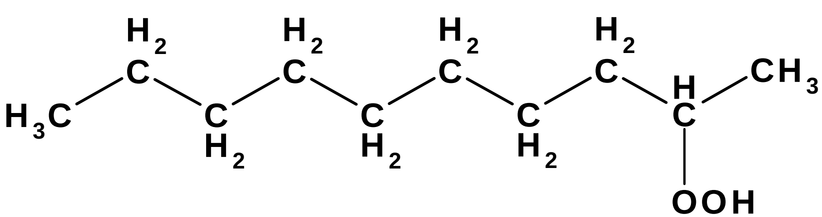
Calculated Data	
$\Delta_f H_{298}$	-402.737
S_{298}	653.220
C_{p298}	270.129
$\Delta_f H_{1000}$	-99.653

Decane-1-hydroperoxide



Calculated Data	
$\Delta_f H_{298}$	-327.857
S_{298}	698.870
C_{p298}	292.168
$\Delta_f H_{1000}$	-8.700

Decane-2-hydroperoxide



Calculated Data	
$\Delta_f H_{298}$	-345.342
S_{298}	644.966
C_{p298}	317.558
$\Delta_f H_{1000}$	-11.971

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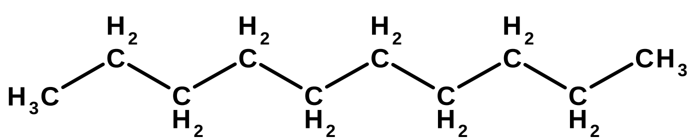
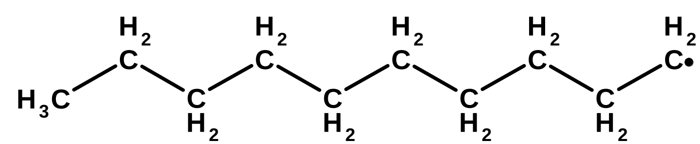
Thermodynamic Database

Molecule	$\Delta_f H_{298}$ kJ/mol	S_{298} J K^{-1} mol^{-1}	C_{p298} J K^{-1} mol^{-1}	$\Delta_f H_{1000}$ kJ/mol
Decane	-252.495	596.739	252.470	29.331
1C10H21	-45.769	582.266	252.207	238.179
2C10H21	-57.215	627.052	246.152	223.399
5C10H21	-55.903	584.729	242.380	222.178

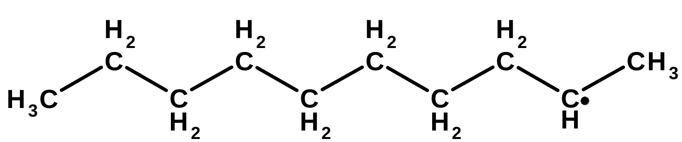
C10H22



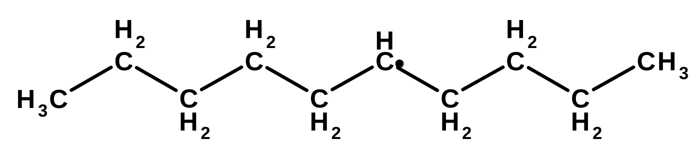
1C10H21



2C10H21



5C10H21



Summary

- Critical reaction paths in the oxidation of aromatic surrogate fuel components have been analyzed and revised rates of reaction proposed.
- Evaluation of proposed rates for the systems studied to date suggest improvements. The latter range from modest to more significant. However, a key point is greater consistency in applied techniques.
- Thermodynamic data bases have been substantially updated for a wide range of compounds and a semi-automatic technique has been formulated and evaluated.
- Further work includes further study of lower temperature toluene and higher pressure 1-methyl napthalene chemistry. Extend work to other alkyl substituted single molecules or surrogate aviation fuel computations
- We expect that substantially updated reaction mechanisms as well as thermodynamic data for target compounds will be made available over the coming year.