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Abstract

The Phenyl + O_2 association results in a chemically activated phenyl-peroxy radical which can dissociate to phenoxy radical + O, undergo intramolecular addition of the peroxy radical to several unsaturated carbon sites or react back to phenyl + O_2. The intramolecular addition channels further react through several paths to ring opening (unsaturated + carbonyl moieties) as well as cyclopentadieny radical + CO_2. Enthalpy ($\Delta H^{\circ}_{f(298)}$), Entropy ($S_{298}$), and heat capacities Cp(T) for species in the decomposition of the ring are evaluated using density functional and *ab initio* calculations and by comparisons to vinyl + O_2 data of Mebel et al, and phenyl + O_2 data of Hadad et al. Isodesmic reaction analysis is used to estimate enthalpy values of the intermediates and well depths of the adducts. High Pressure limit kinetic parameters are obtained from the calculation results using canonical Transition State Theory. Quantum RRK analysis is utilized to obtain k(E) and modified strong collision or master equation analysis is used for evaluation of pressure fall-off in this complex bimolecular, chemical activation, reaction system. Uncertainty in key barriers is discussed, resulting variations in important reaction product ratios are illustrated, and changes in these branching ratios are evaluated with a detailed reaction mechanism.

Introduction

The use and importance of aromatic compounds in fuels contrasts sharply with the limited elementary reaction kinetic data in the literature regarding their combustion kinetics and reaction pathways. A number of experimental and modeling studies on benzene[1-6], toluene[7, 8 and] phenol[9] oxidation, exist in the literature; but it would still be helpful to have more data on species concentration profiles, to understand or evaluate important reaction paths and to validate detailed mechanisms. The above studies show that phenoxy radical is a key intermediate in the gas phase thermal oxidation of aromatics; it is easily formed via abstraction of the weak phenolic hydrogen atom from phenol. Rapid addition of hydroxyl to the aromatic carbons and elimination of H atom10; which occurs even under atmospheric conditions, form the phenol. Work from the Mackie[11] and Louw[12] research groups has also shown that phenoxy radical is an important intermediate in pyrolysis and oxidation of anisole and probably in other phenyl ethers. The thermal decomposition of phenoxy[1, 9,13-16] shows an interesting mechanism in which the bicyclo [3,1,0] hexenone radical is formed and then breaks the cyclic CO--C bond and eliminates carbon monoxide to form the resonance stabilized cyclopentadienyl radical.

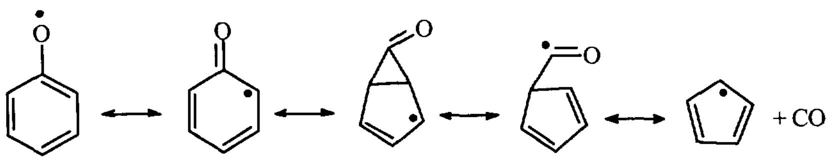

Figure 1, Phenoxy Degradation Reaction Pathway

At higher temperatures this unimolecular C6 -> C5 degradation of the stabilized phenoxy radical is the dominant reaction path.

Venkat et. al[17] published a general reaction scheme for high temperature oxidation of aromatic hydrocarbons that included cyclopentadienyl radical. They postulate that benzene decomposes through the sequence:

C6 => (phenoxy) -> C5 (cyclopentadienyl) -->(+O_2) => O + Cyclic C_5H_5O.

and cyclic C_5H_5O. => linear butadienyl radical (C=C-C=C.) + CO

Wang and Brezinsky[18] recently reported a detailed analysis of cyclopentadienone (C_5H_4O) unimolecular dissociation, which we show is in important product in cyclopentadienyl radical oxidation, where the products were determined to be resonant stabilized cyclobutadienyl radical + CO.

Lovell, et al[1]. reported flow reactor data on benzene combustion at three oxygen concentrations, corresponding to rich, lean and stoichiometric conditions; they showed initial oxygen concentration significantly effects fuel consumption rates along with formation of carbon monoxide and cyclopentadiene. They suggested that phenoxy degradation is major reaction path for both carbon monoxide formation and benzene consumption. Lovell et al [1] also reported experimental data on perturbation of benzene oxidation by NO_2 addition. The benzene oxidation rate doubled in the presence of NO_2 and they suggested additional reaction pathways, including hydroxyl radical association with cyclopentadienyl radical.

A number of researchers have recently published benzene or toluene oxidation models; having made a number of reaction rate modifications to better fit experimental data; but phenyl radical reactions were not analyzed or treated in detail. Bittker[19] published a mechanism, which was based upon previously published reaction paths for ignition delay times plus benzene and toluene loss profiles. Bittker employed a sensitivity code to determine the important reactions and then optimized the fit to the data by adjusting rate constants. Davis et. al[20] modified the Brezinsky groups' mechanism (phenol reactions) to better fit flame speed data. Tan and Frank[21] published a benzene oxidation model and use it for explanation of H and O atom production in their shock tube data. Emdee et al[22] report an updated mechanism for toluene oxidation based on Brezinsky's model[1,17,23]. They indicated that the branching reaction: $C_6H_5CH_3 + O_2 \rightarrow C_6H_5CH_2 + HO_2$ was of major importance. In Emdee et al's[22] toluene mechanism the reactions of resonance stabilized benzyl radical control the reaction at early times.

There are also recent publications that suggest new reaction paths are needed to model aromatic oxidation and combustion.[4,2,23,24] Zhang and Mckinnon et al[4] published an elementary reaction model of high-temperature benzene combustion under fuel rich conditions - near sooting environment. They report that the flame speeds for benzene could not be matched by their model and suggested that some important reaction paths may be missing. Shandross et al[2] reported data from molecular beam experiments on benzene flames and showed that current models strongly overpredicted destruction of phenol at high temperatures. Shandross et al modified the phenol reaction chemistry of Emdee and Brezinsky, of Linstedt and Skevis[3] and of Zhang and Mckinnon to obtain improved results.

The research groups of Glarborg[23], and of Tester et al[24] have recently published benzene mechanisms indicating that the products of phenyl radical with oxygen are uncertain and need to be more clearly identified.

The formation of the very active phenyl radical in combustion systems is important and results from an important class of reactions on aromatic compounds: that is loss a phenyl hydrogen, through abstraction by radical pool species (primarily OH or Cl, H, or O). This occurs even at moderate temperatures in several downstream zones of an incinerator. These radicals will rapidly react with molecular oxygen in the combustion environment to form an energized adduct (chemical activation), which can undergo further reaction through several complex pathways resulting in a number of intermediates and products. The reaction paths, products and kinetics of these radical reactions with O_2 are important to understanding and modeling the oxidation chemistry of these and many other (related) aromatic species.

This study estimates thermodynamic properties of intermediates, transition states and products for destruction of the first ring in this phenyl radical + O_2 reaction system. Thermochemical and kinetic parameters are developed for each elementary reaction path and the flux through each channel as a function of temperature and pressure is estimated using bimolecular chemical activation analysis. An elementary reaction mechanism is constructed to model experimental data performed at one atmosphere pressure, ambient conditions, in a combustor and in higher pressure turbine systems, as well as at very high pressure oxidation in supercritical water.

The approach starts with and extends a mechanism initially proposed by Carpenter[25], who studied the reaction of phenyl radicals with molecular oxygen (C_6H_5) using semi-empirical calculations. Mebel et al. furthered the work of Carpenter on this vinyl system.[27] The research group of Hadad have further studied and estimated Gibbs energy of reactants, TSTs and products in this phenyl + O_2 reaction system using B3LYP density functional calculations[27-30]. The association reaction results in a chemically activated phenylperoxy radical which can then dissociate to a phenoxy radical + O atom or undergo unimolecular addition of the peroxy radical to the ipso carbon. This intramolecular addition channel further reacts through several paths to ring opening and ring expansion products; which are at much lower energies and are also chemically activated species.

Enthalpy ($\Delta H^{\circ}_{f(298)}$), Entropy S_{298}, and heat capacities Cp(T) for species in the decomposition of the first ring are evaluated using density functional calculations and by comparisons to vinyl + O_2 calculation data of Mebel et al, and phenyl + O_2 data of Hadad et al. We show that the vinyl radical is a good model for phenyl, where high level calculations on the smaller vinyl system can be used to calibrate *ab initio* and density functional calculations on the phenyl system. Isodesmic reaction analysis is used to estimate enthalpy values of the intermediates and well depths of the adduct.

Kinetic Calculations

Unimolecular dissociation and isomerization reactions of the chemically activated and stabilized adducts resulting from addition or combination reactions are analyzed by first constructing potential energy diagrams. Thermodynamic parameters, $H_f^o{}_{(298)}$, $S_f^o{}_{(298)}$, Cp(T), reduced vibration frequency sets, and Lennard Jones parameters for species in each reaction path are presented.

High-pressure rate constants for each channel are obtained from literature or referenced estimation techniques. Kinetics parameters for unimolecular and bimolecular (chemical activation) reactions are then calculated using multi-frequency QRRK analysis for k(E)[31-33] The master equation formalism of Gilbert et al[34] is used for fall-off with the steady state assumption on the energized adduct(s).

Enthalpies and E_a's, in the text and in PE diagrams are at 298 K, while those in the tables listing data input to the chemical activation reactions are for 1000 K, which we select as representative of modeled combustion experiments.

Recent Modifications to the Quantum RRK Calculation Include:

a. Fall off is analyzed with master equation analysis.
b. Use of a manifold of three frequencies plus incorporation of one external rotation for the density of states, $\rho(E)/Q$ and in calculation of k(E) and of F(E).
c. The collision efficiency βc is calculated with the calculated FE(T) factor instead of the previously assigned 1.15 value. βc is now calculated from Gilbert et al[34], Eqn. 4.7.
d. The Leonard-Jones collision frequency Z_{LJ} is now calculated by $Z_{LJ} = Z\,\Omega$ integral[35-37] obtained from fit of Reid et al[37].

The QRRK analysis with the "modified strong collision approach" and constant FE for fall-off has been used to analyze a variety of chemical activation reaction systems, Westmoreland et al[31, 38], Dean et al[39], Bozzelli et al[40-42]. There are a number of recent publications by other researchers, that utilize the QRRK formalism with a more exact calculation of FE (as in this study) in the modified strong collision analysis [43-48] or utilize just a QRRK formalism.[49-50] Bauman notes its suitability for explanation of product ratios in ion molecule reaction systems[49]. It is shown to yield reasonable results in these applications, and provides a framework by which the effects of temperature and pressure can be evaluated.

Computational Methods

All *ab initio* calculations are performed using the Gaussian 94 or Gaussian 98 program suites.[b13] The structural parameters are fully optimized at B3LYP/6-311G(d,p) or B3LYP/6-31g(d,p) levels of theory. Harmonic vibration frequencies and scaled zero-point vibrational energies (ZPVE) are computed at the same level. The optimized geometry parameters are used to obtain total electronic energies in B3LYP/6-311G(d,p), B3LYP/6-311+G(3df,2p), QCISD(T)/6-31G(d,p) and CBSQ//B3LYP/6-31G(d,p) single point calculations.[b14-b16] Calculation levels higher that the B3LYP/6-311g(d,p) were only used for smaller molecules in this Phenyl + O_2 study. Differences between density functional and higher level calculations on smaller molecules were used to calibrate the density functional calculations as applied to larger phenyl-O2 adduct system.

B3LYP/6-31G(d,p) is chosen because it is commonly used and is reported to yield accurate geometry and reasonable energies.[b17-b18] Curtiss et al.[b19] recently reported that G3 (MP2) with B3LYP/6-31G(d) geometries yield overall enthalpy values for alkyl hydrocarbons show a low overall deviation from experimental values. Durant[b17, b20] has compared density functional calculations BHandH and B3LYP with MP2 and Hartree-Fock methods for geometry and vibration frequencies. He reports that these density functional methods provide excellent geometry and vibration frequencies, relative to MP2 at reduced computation expense. Petersson[b21] et al. compared energy of density functional methods of B3LYP/6-311+G(3df,2p)//B3LYP/6-31G with G2 study, and his CBS calculation methods and report that they have been successful for a wide range of molecules. Wong and Radom[b22,b23] indicated the B3LYP/6-31G(d,p) geometry corresponds closely to QCISD(T)/6-31G(d,p). Comparison of calculation results from B3LYP/6-31G(d,p) against data from higher calculation levels in use of working reaction for $\Delta H_f^o{}_{298}$, will provide some calibration of the B3LYP/6-31G(d,p) values with similar working reactions, for larger molecules, where this may be one of the few available calculation methods.

B3LYP/6-311+G(3df,2p) is chosen to evaluate if this large basic set results in an improvement to the above commonly used density functional calculation method.[b18] QCISD(T)/6-31G(d,p) is a configuration interaction method; but with a small, economical basis set.[b22,b24] CBS-Q calculation is a high level composite method with empirical correction; it is reported to be nearly equivalent to QCISD(T)/6-311+G(3df,2p).[b16,b25] The CBS-Q method[b26] attempts to approximate the energy of a species at the infinite basis set limit by an extrapolation of the energies of pair natural orbital at the MP2 level. The effects of going from MP2 to QCISD(T) are accounted for with an additivity scheme. For the open-shell systems, there is also a correction for spin contamination in the unrestricted Hartree-Fock wave function. The CBS-Q method has been shown to yield reliable $\Delta H_f^o{}_{298}$ values for small (C_1 to C_3) molecules.[b26]

Thermodynamic Properties Using *ab initio* Calculations

Enthalpy, $\Delta H_f^o{}_{298}$, entropy, $S^o{}_{298}$ and heat capacities $C_p(T)$, ($300 < T/K < 1500$) are determined primarily with Density Functional B3LYP/6-311G(d,p), B3LYP/6-31+G(d,p) calculation methods. Comparisons to higher level calculations on the vinyl–OO system are made for the phenyl peroxy radical, and the important transition state to Phenoxy + O atom.

Molecular structures and vibration frequencies are determined at the B3LYP/6-31G(d,p) density functional calculation level. Vibration frequencies are scaled [b27] by 0.9806 for zero point energies (ZPVE). Enthalpies of formation are determined at each calculation level using the enthalpy of reaction ($\Delta H_r^o{}_{298}$) with known enthalpies of other reactants in each of isodesmic reaction.[b28-b29] Barriers for intramolecular rotation about the two carbon-oxygen or carbon – carbon single bonds are analyzed versus torsional angle using B3LYP/6-31G(d,p) and B3LYP/3-21G levels of calculation.

Transition states are determined from the thermodynamic properties determined in the calculations and Cannonical Transition State Theory.

Input Data Requirements for QRRK Calculation

High pressure limit pre-exponential factor (Arrhenius A factor, A(T)) for the bimolecular addition / combination reactions is obtained from calculation and literature data. A factors for isomerizations are obtained from cannonical transition state theory and the calculated saddle point transition state structure and vibration frequencies. Entropies of hindered internal rotors are included in the analysis. Enthalpies of the adducts are from isodesmic reaction analysis or isodesmic reaction analysis with group balance if feasible, as is the case with phenyl peroxide radical. Activation energies come from averaged enthalpy differences between calculated enthalpies of the reactant and product adducts and the transition state. We feel the use of isodesmic reaction values for adduct enthalpies provides in more accurate estimate of the transition state enthalpies.

Results and Discussion – Potential energy Diagram and Kinetic Parameters

Enthalpies of Phenyl hydroperoxide and phenyl peroxy radical were analyzed using the isodesmic reactions as illustrated in Table 1.

A potential energy diagram for the reaction of phenyl radical + O_2 is illustrated in Figure 2.

Nomenclature in this figure: **PH** represents phenyl, **Y** represents a cyclic structure, **D** is a double bond (CDO is C=O), A • represents a radical site on the structure, and **j** represents a radical site in the name. Several resonant structures are often present for a given species. The high pressure rate constants, as a function of temperature (represented as $k = A\ T^n \exp(-Ea/RT)$ with Ea in kcal/mole), delta E down and energy grain in the master equation analysis for the reaction system; and Lennard Jones parameters and vibration sets for the reaction species are illustrated in the input file for the chemical activation reaction system – Appendix.

There are four reactions of high importance in the chemical activation (bimolelcular reaction) of phenyl + O_2. i. formation of phenyl peroxy radical (stabilization), with three reactions of the activated of phenyl-peroxy radical; all of these have barriers lower than or similar to that of the phenyl + O_2 inlet channel (reactants). These three important reaction paths of the activated phenyl peroxy are: ii, dissociation to phenoxy radical plus oxygen atom (PhO. + O), iii. reaction to isomer C6jYOO with the further reaction of this isomer to two product sets through the cyclic oxy-pinoxy radical (YOC6jDO) , and iv. reaction back to phenyl + O_2. There are two major product sets for the forward reaction cyclic oxy-pinoxy radical, iii-a, a ring opening (RO) channel to RODC6jDO and iii-b, a ring closure, formation of a bicyclic Y5jYO4DO. The Y5jYO4DO undergoes further beta scission to open the newly formed 4 member ring, forming to a cyclic cyclopentadienyl carboxy radical, and this carboxy radical dissociates (elimination reaction) to CO_2 + cyclopentadienyl radical.

Phenylperoxy radical reactions to phenoxy + O and to back to phenyl + O_2 have loose transition states, but higher barriers than reaction to oxypinoxy radical, which has a tight transition state. A comparison of the calculated potential curves for this dissociation reaction versus PhO-O bond distance with the corresponding bond cleavage for vinylperoxy radical is illustrated in figure 3. The B3LYP calculated values are similar to those of the vinyl-OO reaction to vinoxy + O atom of Mebel et al.[27] The MP2 calculations show a significant barrier, which reverts to lower values with higher level composite calculation methods.

The PhO—O potential diagram of figure 2 illustrates that the density functional calculations illustrate the same pattern for both reaction systems, that is there is a very small or no barrier in addition to the reaction endothermicity, for dissociation of phenylperoxy to PhO + O. The density functional calculations are also similar to those determined by Mebel and Lin[27] and we conclude this dissociation is somewhat lower than the barrier previously estimated[28-30].

Results and Discussion - Chemical Activation Reaction – Phenyl + O_2

Figures 4 and 5 illustrate the reaction product profiles as a function of temperature and of pressure, respectively for the values determined and recommended in this study. The contribution to the phenoxy + O atom channel is markedly increased. The reactions to ring opening and dissociation back to reactants, phenyl + O_2 are both decreased significantly; but both are still important channels. In this chemical activation reaction the ring opening product, RODC6jDOP (O=Cj—C=C—C=C-C=O), is formed with 76 kcal/mole of excess energy. We treat this as an energized adduct and allow dissociation (beta scission reaction) to CO + a vinylic linear C_5H_5O radical (O=C--C=C--C=C•). This vinylic radical will further beta scission (unzip) to two acetylenes + HC.=O radical or rapidly react with molecular oxygen.

Results and Discussion - Unimolecular Dissociation of PHOO

Figure 6 illustrates the dissociation of the stabilized phenyl peroxy adduct to the several important reaction channels as a function of temperature at 1 atm. The top figure shows the competition between the two loose transition state channels: Phenoxy + O atom and Phenyl + O_2; the lower energy channel to phenoxy is dominant in this comparison. The bottom figure shows a more complete analysis with isomer C6jYOO is the overall dominant channel. The important reaction of this C6jYOO isomer is to YOC6jDO and subsequently to the two other important (final) dissociation products RODC6jDO and cyclopentadienyl and CO_2. For dissociation of this phenylperoxy adduct two channels are competitive:

Phenoxy + O atom, and ring opening to CO + O=C--C=C--C=C•.

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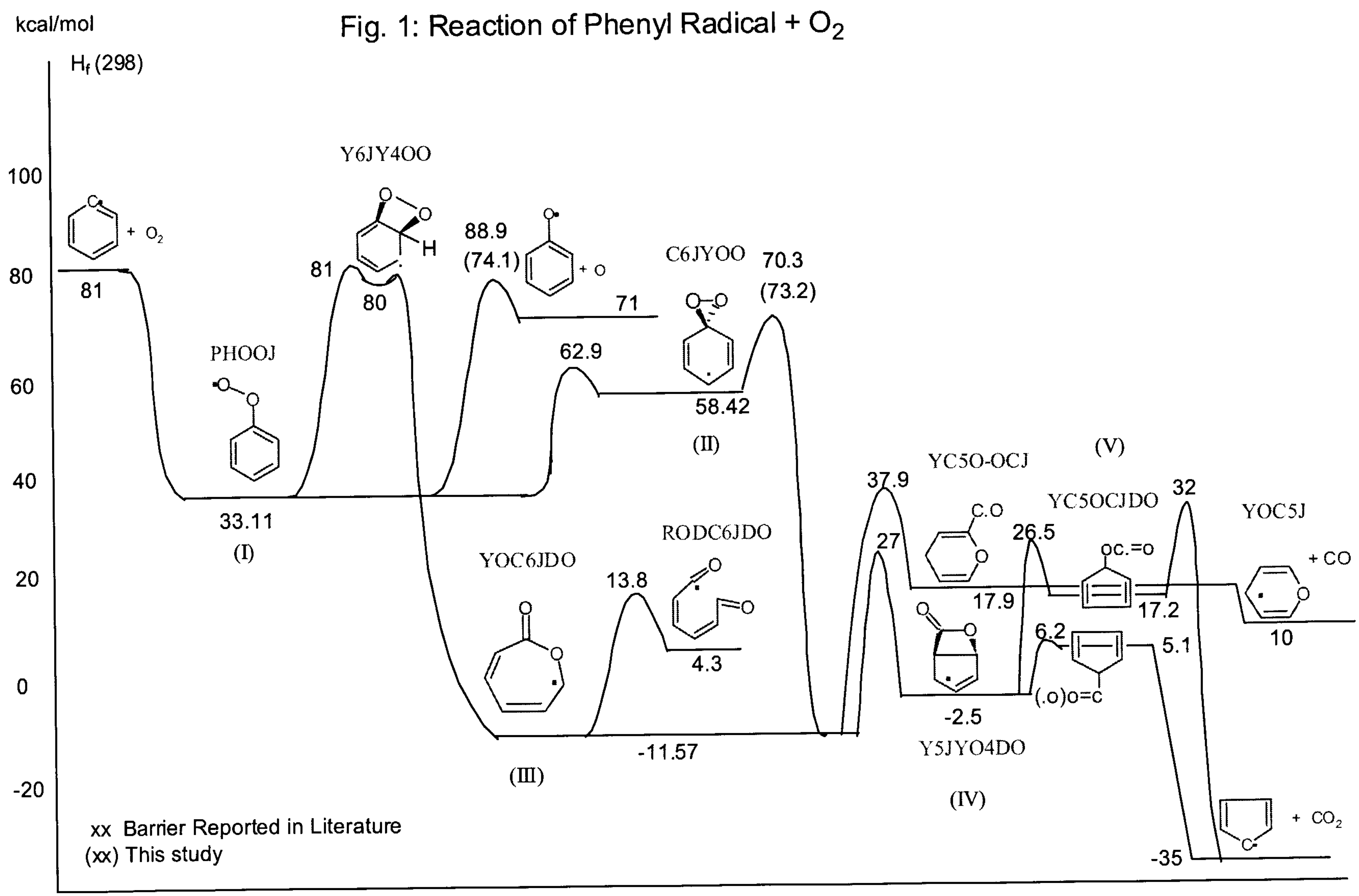
Table 1 - Standard Enthalpies of Formation (298 K, kcal/mole)

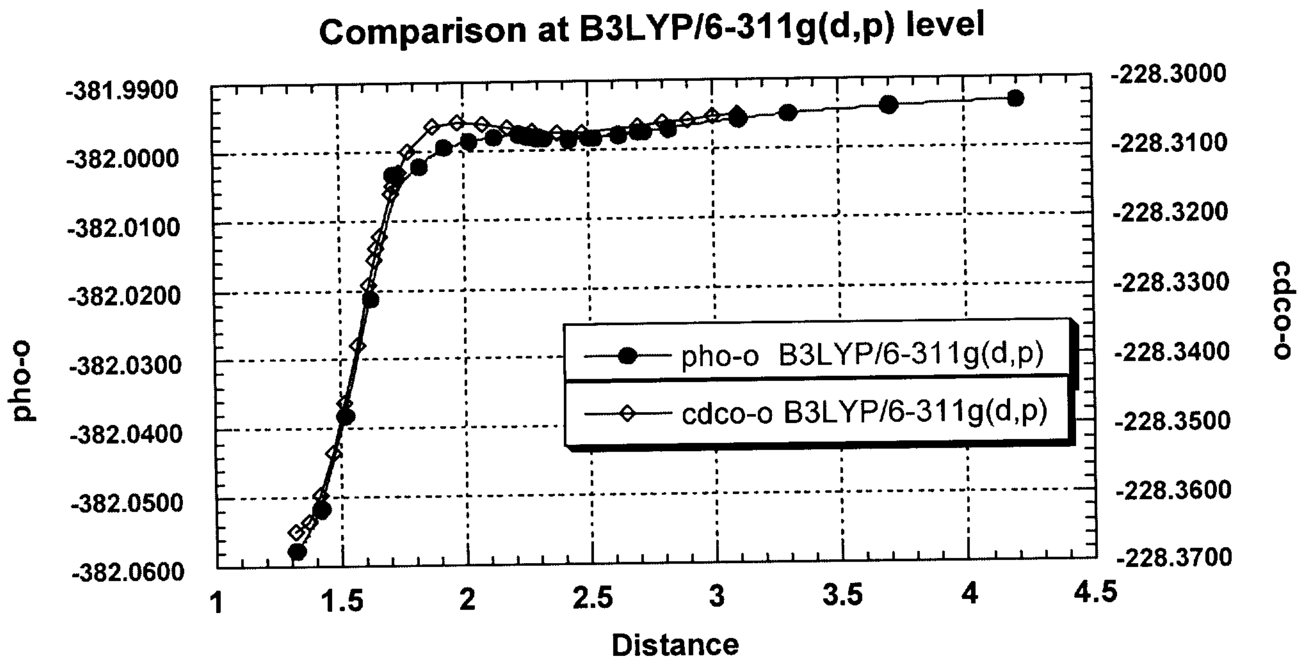
PHOOH + CH_3-CH_3 => Ph + CH_3-CH_2OOH	**PHOOH = -3.377**
PHOOH + CH_2=CH_2 => Ph + CH_2=CHOOH	**PHOOH = -2.149**
	Average = -2.763
PHOO. + CH_2=CHOOH => PHOOH +CH_2=CHOO.	**PHOO. = 31.77**
PHOO. + CH_3-CH_2OOH => PHOOH + CH_3-CH_2OO.	**PHOO. = 30.83**
	Average = 31.30
PHCOOH + CH_3-CH_3 => Toluene + CH_3-CH_2OOH	**PHCOOH = -8.13**
PHCOOH + CH_2=CH-CH_3=> Toluene + CH_2=CH-CH_2OOH	**PHCOOH = -7.19**
	Average = -8.02
PHCOO. + CH_3OOH => PHCOOH +CH_3OO.	**PHCOO. = 29.81**



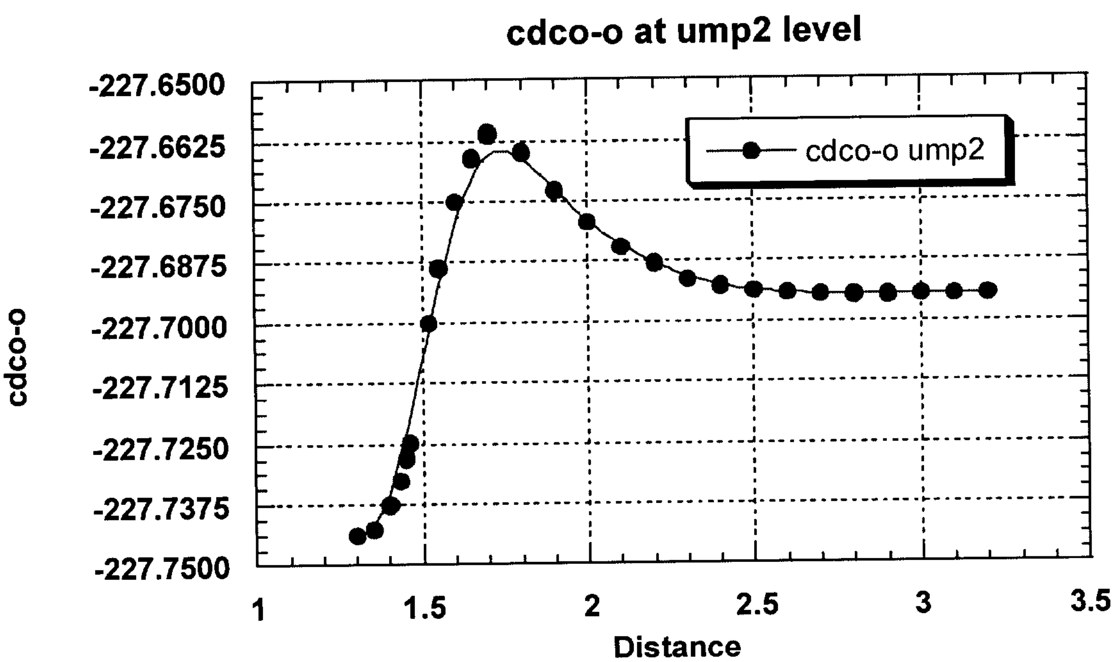
kcal/mol
Fig. 1: Reaction of Phenyl Radical + O_2
H_f (298)
100
80
60
40
20
0
-20
+ O_2
81
PHOOJ
33.11
(I)
Y6JY4OO
81
80
88.9
(74.1)
+ O
71
62.9
C6JYOO
70.3
(73.2)
58.42
(II)
YOC6JDO
13.8
RODC6JDO
4.3
-11.57
(III)
37.9
27
YC5O-OCJ
C.O
17.9
-2.5
Y5JYO4DO
(IV)
(V)
YC5OCJDO
26.5
oc.=o
6.2
(.o)o=c
17.2
5.1
32
YOC5J
+ CO
10
+ CO_2
-35
xx Barrier Reported in Literature
(xx) This study

Fig. 2

Fig. 3



Comparison at B3LYP/6-311g(d,p) level
-381.9900
-382.0000
-382.0100
-382.0200
-382.0300
-382.0400
-382.0500
-382.0600
pho-o
-228.3000
-228.3100
-228.3200
-228.3300
-228.3400
-228.3500
-228.3600
-228.3700
cdco-o
pho-o B3LYP/6-311g(d,p)
cdco-o B3LYP/6-311g(d,p)
1
1.5
2
2.5
3
3.5
4
4.5
Distance



cdco-o at ump2 level
-227.6500
-227.6625
-227.6750
-227.6875
-227.7000
-227.7125
-227.7250
-227.7375
-227.7500
cdco-o
cdco-o ump2
1
1.5
2
2.5
3
3.5
Distance

Fig. 4

(Mar 2001 (chemast) PH + O_2 => Products PhO—O Low)

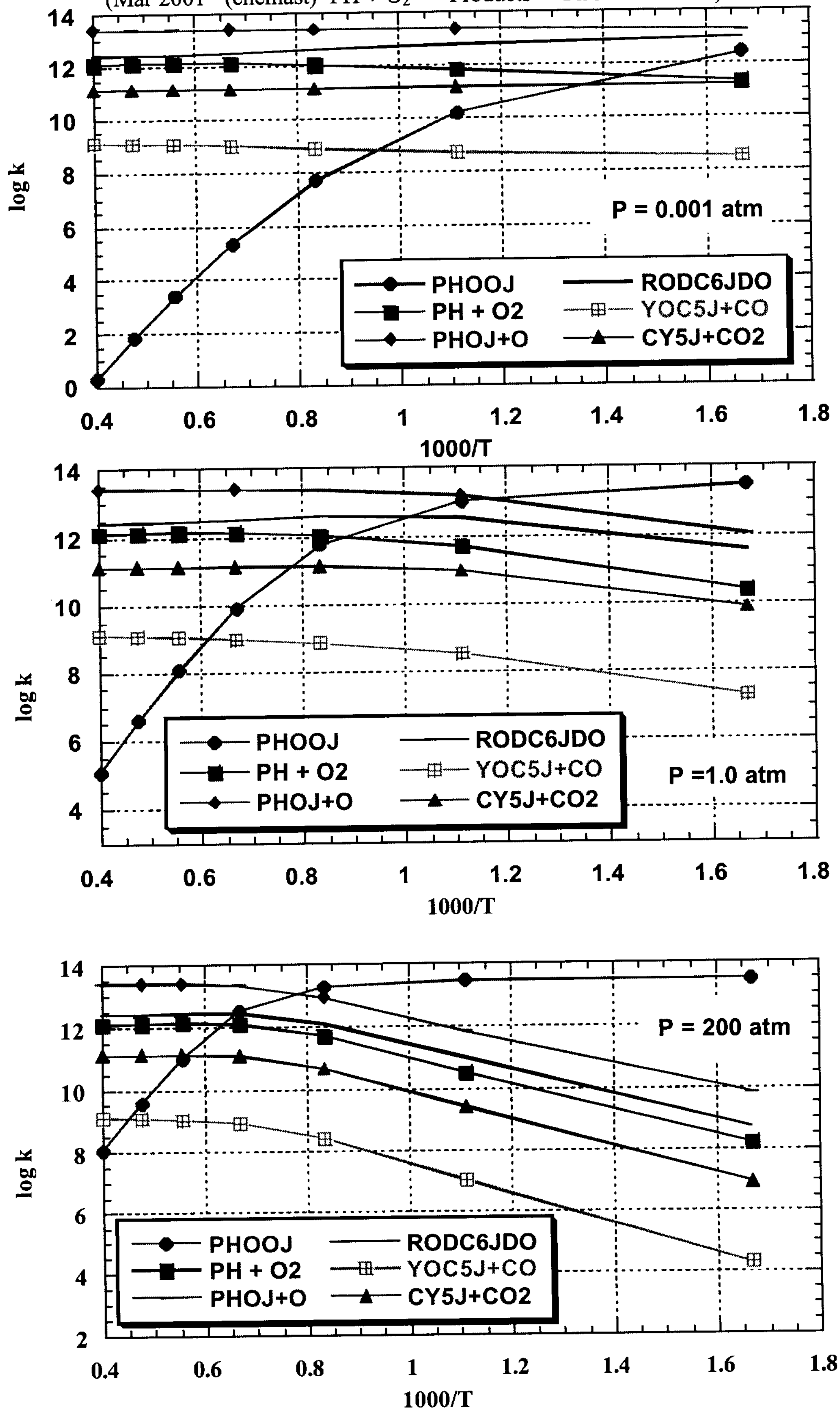


Fig. 5
(Mar 2001 (chemast) PH + O_2 => Products Low PhO-O)

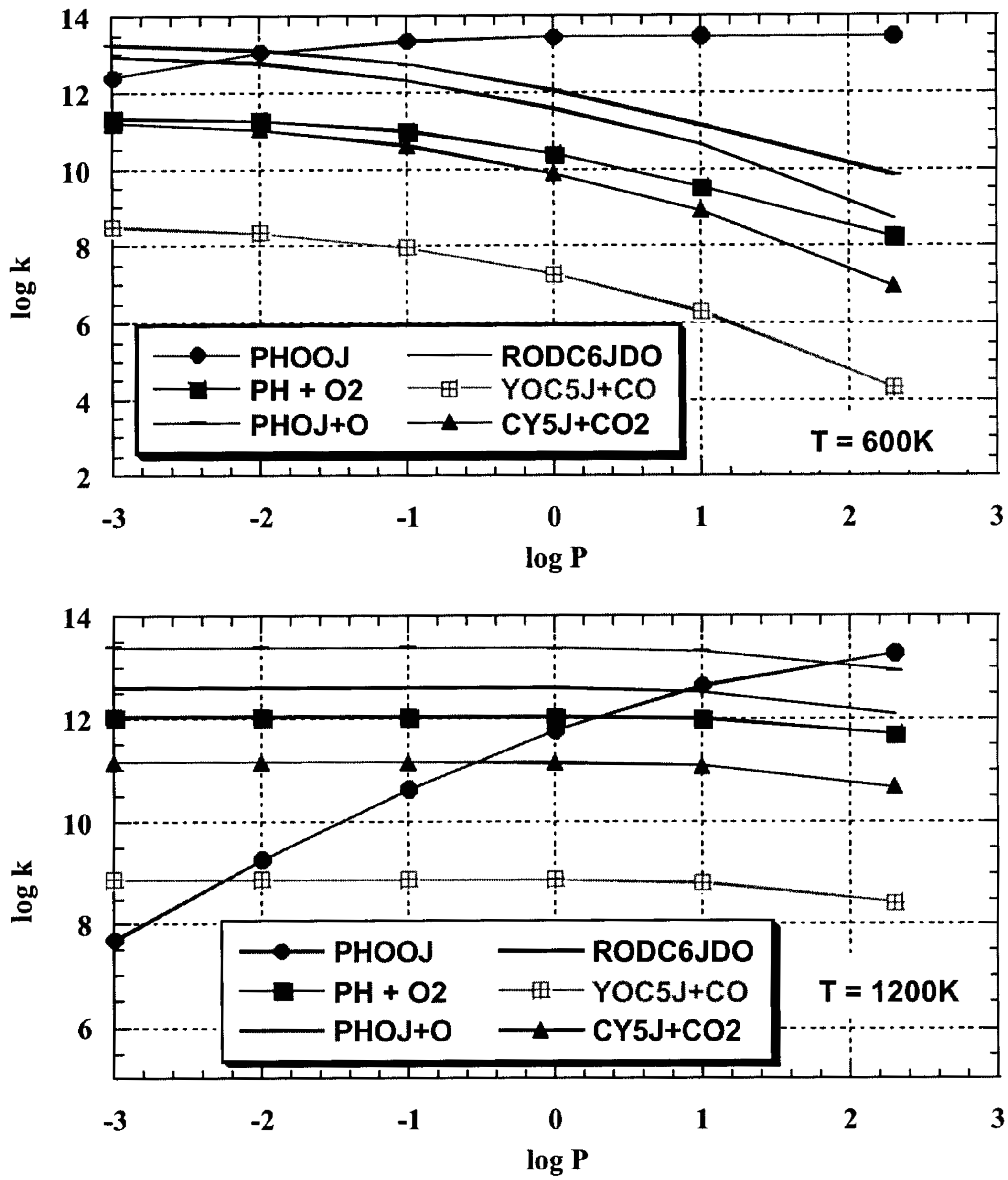
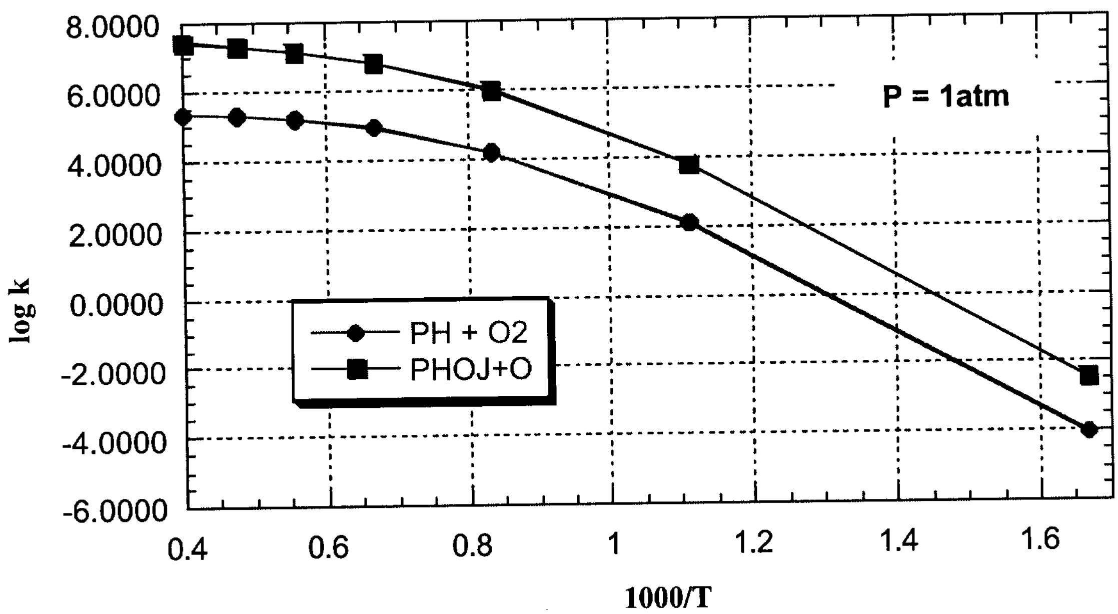
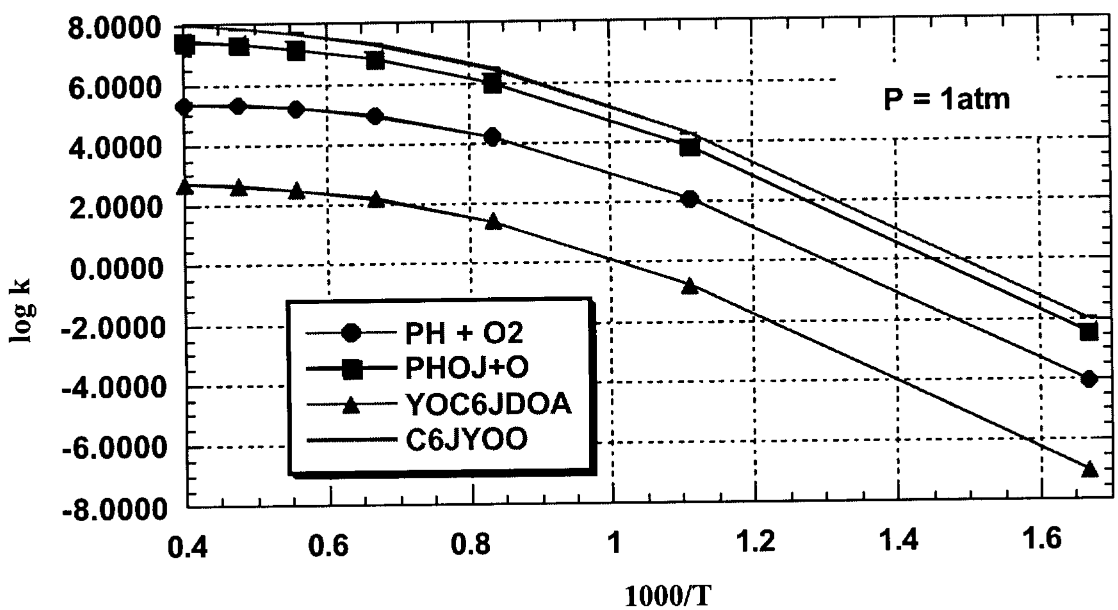


Fig. 6: Dissociation for PHOOJ





Appendix

APPENDIX

Mar 2001 (chemast) PH + O2 => Products low for sensitivity Low jwb / N sebar

ChemMaster chemact output for mac spreadsheet

reactants: PH + O2

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1.00E-03	600	1.667	12.398	11.325	8.38	13.259	14.324	3.923	14.305	12.961	-6.501	12.954	8.492	4.401	11.197	-10.624	11.194	8.743	8.907	-11.5	8.582	8.629	13.474	13.477
1.00E-03	900	1.111	10.187	11.815	8.927	13.366	13.851	1.435	13.812	12.784	-7.02	12.773	8.689	5.581	11.171	-10.684	11.166	9.007	9.16	-11.522	8.899	8.815	13.468	13.477
1.00E-03	1200	0.833	7.698	12.045	9.204	13.391	13.486	-1.107	13.42	12.632	-7.415	12.617	8.87	6.417	11.163	-11.254	11.153	9.245	9.389	-12.012	9.173	8.982	13.461	13.477
1.00E-03	1500	0.667	5.354	12.147	9.347	13.402	13.242	-3.476	13.149	12.528	-8.101	12.509	8.995	6.876	11.161	-11.543	11.146	9.404	9.543	-12.001	9.353	9.094	13.456	13.477
1.00E-03	1800	0.556	3.41	12.163	9.401	13.407	13.121	-5.43	13.009	12.478	-8.388	12.457	9.06	7.082	11.161	-11.642	11.142	9.483	9.619	-12.384	9.441	9.146	13.456	13.477
1.00E-03	2100	0.476	1.867	12.146	9.418	13.41	13.069	-6.976	12.947	12.458	-8.713	12.436	9.095	7.182	11.16	-11.678	11.14	9.521	9.656	-12.008	9.485	9.169	13.456	13.477
1.00E-03	2500	0.4	0.284	12.109	9.42	13.413	13.041	-8.545	12.913	12.449	-8.998	12.427	9.123	7.254	11.16	-12.284	11.138	9.547	9.681	-12.707	9.516	9.181	13.458	13.477

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1.00E-02	600	1.667	13.039	11.25	8.302	13.115	14.079	4.565	14.057	12.767	-5.753	12.759	8.344	4.349	11.026	-9.819	11.023	8.605	8.768	-10.692	8.449	8.484	13.475	13.477
1.00E-02	900	1.111	11.438	11.813	8.925	13.363	13.849	2.688	13.811	12.779	-6.021	12.769	8.686	5.58	11.167	-9.687	11.162	9.004	9.157	-10.526	8.896	8.812	13.468	13.477
1.00E-02	1200	0.833	9.266	12.045	9.204	13.391	13.487	0.46	13.422	12.632	-6.415	12.617	8.87	6.417	11.163	-10.254	11.153	9.244	9.389	-11.012	9.173	8.982	13.461	13.477
1.00E-02	1500	0.667	7.028	12.147	9.347	13.402	13.243	-1.802	13.149	12.528	-7.1	12.509	8.995	6.876	11.161	-10.543	11.146	9.404	9.543	-11.001	9.353	9.094	13.456	13.477
1.00E-02	1800	0.556	5.124	12.163	9.401	13.407	13.122	-3.717	13.01	12.478	-7.388	12.457	9.06	7.082	11.161	-10.642	11.142	9.483	9.619	-11.384	9.441	9.146	13.456	13.477
1.00E-02	2100	0.476	3.605	12.146	9.418	13.41	13.069	-5.239	12.947	12.458	-7.713	12.436	9.095	7.182	11.16	-10.678	11.14	9.521	9.656	-11.008	9.485	9.169	13.456	13.477
1.00E-02	2500	0.4	2.047	12.109	9.42	13.413	13.041	-6.794	12.913	12.449	-7.998	12.427	9.123	7.254	11.16	-11.284	11.138	9.547	9.681	-11.707	9.516	9.181	13.458	13.477

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1.00E-01	600	1.667	13.352	10.98	8.023	12.728	13.556	4.888	13.531	12.31	-0.911	12.301	7.959	4.14	10.603	-9.239	10.6	8.236	8.397	-10.106	8.089	8.103	13.476	13.477
1.00E-01	900	1.111	12.386	11.797	8.909	13.332	13.793	3.637	13.753	12.737	-4.481	12.726	8.66	5.574	11.133	-8.725	11.128	8.981	9.134	-9.554	8.874	8.786	13.468	13.477
1.00E-01	1200	0.833	10.628	12.044	9.203	13.39	13.491	1.824	13.426	12.632	-5.413	12.617	8.869	6.416	11.163	-9.254	11.153	9.244	9.388	-10.013	9.172	8.982	13.461	13.477
1.00E-01	1500	0.667	8.535	12.147	9.347	13.402	13.243	-0.294	13.15	12.528	-6.098	12.509	8.995	6.876	11.161	-9.543	11.146	9.404	9.543	-10.001	9.353	9.094	13.456	13.477
1.00E-01	1800	0.556	6.672	12.163	9.401	13.407	13.122	-2.168	13.01	12.478	-6.387	12.457	9.06	7.082	11.161	-9.642	11.142	9.483	9.619	-10.383	9.441	9.146	13.456	13.477
1.00E-01	2100	0.476	5.173	12.146	9.418	13.41	13.069	-3.671	12.947	12.458	-6.713	12.436	9.095	7.182	11.16	-9.678	11.14	9.521	9.656	-10.008	9.485	9.169	13.456	13.477
1.00E-01	2500	0.4	3.632	12.109	9.42	13.413	13.041	-5.211	12.913	12.449	-6.998	12.427	9.122	7.254	11.16	-10.284	11.138	9.547	9.681	-10.707	9.516	9.181	13.458	13.477

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1.00E+00	600	1.667	13.455	10.386	7.422	12.034	12.763	5.057	12.735	11.564	5.841	11.555	7.269	3.626	9.883	-8.961	9.879	7.561	7.72	-4.565	7.42	7.417	13.477	13.477
1.00E+00	900	1.111	13.02	11.705	8.814	13.188	13.569	4.293	13.525	12.558	3.48	12.546	8.534	5.528	10.981	-7.894	10.975	8.865	9.017	-7.865	8.763	8.662	13.47	13.477
1.00E+00	1200	0.833	11.778	12.039	9.198	13.382	13.484	2.983	13.419	12.623	0.503	12.608	8.863	6.414	11.154	-8.262	11.144	9.238	9.382	-9.02	9.166	8.975	13.461	13.477
1.00E+00	1500	0.667	9.911	12.147	9.347	13.402	13.246	1.087	13.154	12.529	-2.928	12.51	8.994	6.876	11.161	-8.541	11.146	9.404	9.543	-9.001	9.353	9.093	13.456	13.477
1.00E+00	1800	0.556	8.099	12.163	9.401	13.407	13.122	-0.738	13.01	12.478	-5.291	12.457	9.06	7.081	11.161	-8.642	11.142	9.483	9.619	-9.383	9.441	9.146	13.456	13.477
1.00E+00	2100	0.476	6.619	12.146	9.418	13.41	13.069	-2.223	12.947	12.458	-5.712	12.436	9.095	7.182	11.16	-8.678	11.14	9.521	9.656	-9.008	9.485	9.169	13.456	13.477
1.00E+00	2500	0.4	5.092	12.109	9.42	13.413	13.041	-3.75	12.913	12.449	-5.998	12.427	9.122	7.254	11.16	-9.283	11.138	9.547	9.681	-9.707	9.516	9.181	13.458	13.477

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1.00E+01	600	1.667	13.475	9.518	6.551	11.123	11.815	5.293	11.785	10.632	9.045	10.612	6.29	2.716	8.912	-6.015	8.908	6.582	6.741	0.521	6.441	6.439	13.477	13.477
1.00E+01	900	1.111	13.347	11.394	8.497	12.794	13.069	4.697	13.017	12.115	8.241	12.102	8.165	5.312	10.574	-7.302	10.567	8.513	8.662	-1.861	8.417	8.297	13.474	13.477
1.00E+01	1200	0.833	12.651	12	9.157	13.322	13.389	3.891	13.321	12.547	6.586	12.532	8.811	6.394	11.091	-7.333	11.081	9.191	9.335	-4.169	9.121	8.924	13.462	13.477
1.00E+01	1500	0.667	11.151	12.144	9.344	13.399	13.252	2.345	13.161	12.528	3.906	12.51	8.991	6.872	11.158	-7.536	11.144	9.4	9.539	-6.736	9.349	9.09	13.456	13.477
1.00E+01	1800	0.556	9.417	12.163	9.401	13.407	13.125	0.59	13.014	12.479	1.119	12.458	9.059	7.08	11.16	-7.641	11.142	9.482	9.618	-8.336	9.44	9.145	13.456	13.477
1.00E+01	2100	0.476	7.955	12.146	9.418	13.41	13.07	-0.881	12.949	12.458	-1.198	12.436	9.095	7.181	11.16	-7.678	11.14	9.52	9.656	-8.008	9.484	9.168	13.456	13.477
1.00E+01	2500	0.4	6.443	12.109	9.42	13.413	13.042	-2.396	12.914	12.449	-3.608	12.427	9.122	7.253	11.159	-8.281	11.138	9.546	9.681	-8.706	9.515	9.181	13.458	13.477

P (atm)	T (K)	1000/T	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
2.00E+02	600	1.667	13.477	8.242	5.274	9.837	10.521	6.105	10.492	9.333	9.208	8.726	4.295	0.724	6.951	0.122	6.948	4.575	4.734	3.208	4.394	4.445	13.477	13.477
2.00E+02	900	1.111	13.465	10.51	7.608	11.831	12.011	5.037	11.954	11.105	10.422	10.992	7.044	4.355	9.439	-0.852	9.431	7.402	7.55	2.93	7.308	7.179	13.477	13.477
2.00E+02	1200	0.833	13.285	11.697	8.851	12.949	12.907	4.584	12.829	12.123	10.424	12.099	8.423	6.122	10.673	-1.951	10.661	8.817	8.959	1.183	8.751	8.539	13.47	13.477
2.00E+02	1500	0.667	12.51	12.101	9.3	13.352	13.207	3.707	13.117	12.48	9.185	12.461	8.924	6.807	11.096	-3.692	11.081	9.333	9.472	-0.441	9.281	9.023	13.458	13.477
2.00E+02	1800	0.556	11.002	12.156	9.395	13.406	13.139	2.156	13.03	12.483	6.94	12.462	9.044	7.052	11.153	-5.995	11.135	9.464	9.601	-2.53	9.421	9.13	13.456	13.477
2.00E+02	2100	0.476	9.574	12.143	9.415	13.41	13.078	0.708	12.957	12.461	4.865	12.439	9.086	7.163	11.156	-6.364	11.137	9.51	9.646	-4.435	9.474	9.16	13.457	13.477
2.00E+02	2500	0.4	8.077	12.108	9.418	13.413	13.045	-0.8	12.918	12.451	2.663	12.428	9.117	7.241	11.157	-6.941	11.136	9.54	9.674	-6.42	9.509	9.176	13.458	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
600	-3	12.398	11.325	8.38	13.259	14.324	3.923	14.305	12.961	-6.501	12.954	8.492	4.401	11.197	-10.624	11.194	8.743	8.907	-11.5	8.582	8.629	13.474	13.477
600	-2	13.039	11.25	8.302	13.115	14.079	4.565	14.057	12.767	-5.753	12.759	8.344	4.349	11.026	-9.819	11.023	8.605	8.768	-10.692	8.449	8.484	13.475	13.477
600	-1	13.352	10.98	8.023	12.728	13.556	4.888	13.531	12.31	-0.911	12.301	7.959	4.14	10.603	-9.239	10.6	8.236	8.397	-10.106	8.089	8.103	13.476	13.477
600	0	13.455	10.386	7.422	12.034	12.763	5.057	12.735	11.564	5.841	11.555	7.269	3.626	9.883	-8.961	9.879	7.561	7.72	-4.565	7.42	7.417	13.477	13.477
600	1	13.475	9.518	6.551	11.123	11.815	5.293	11.785	10.632	9.045	10.612	6.29	2.716	8.912	-6.015	8.908	6.582	6.741	0.521	6.441	6.439	13.477	13.477
600	2.301	13.477	8.242	5.274	9.837	10.521	6.105	10.492	9.333	9.208	8.726	4.295	0.724	6.951	0.122	6.948	4.575	4.734	3.208	4.394	4.445	13.477	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
900	-3	10.187	11.815	8.927	13.366	13.851	1.435	13.812	12.784	-7.02	12.773	8.689	5.581	11.171	-10.684	11.166	9.007	9.16	-11.522	8.899	8.815	13.468	13.477
900	-2	11.438	11.813	8.925	13.363	13.849	2.688	13.811	12.779	-6.021	12.769	8.686	5.58	11.167	-9.687	11.162	9.004	9.157	-10.526	8.896	8.812	13.468	13.477
900	-1	12.386	11.797	8.909	13.332	13.793	3.637	13.753	12.737	-4.481	12.726	8.66	5.574	11.133	-8.725	11.128	8.981	9.134	-9.554	8.874	8.786	13.468	13.477
900	0	13.02	11.705	8.814	13.188	13.569	4.293	13.525	12.558	3.48	12.546	8.534	5.528	10.981	-7.894	10.975	8.865	9.017	-7.865	8.763	8.662	13.47	13.477
900	1	13.347	11.394	8.497	12.794	13.069	4.697	13.017	12.115	8.241	12.102	8.165	5.312	10.574	-7.302	10.567	8.513	8.662	-1.861	8.417	8.297	13.474	13.477
900	2.301	13.465	10.51	7.608	11.831	12.011	5.037	11.954	11.105	10.422	10.992	7.044	4.355	9.439	-0.852	9.431	7.402	7.55	2.93	7.308	7.179	13.477	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1200	-3	7.698	12.045	9.204	13.391	13.486	-1.107	13.42	12.632	-7.415	12.617	8.87	6.417	11.163	-11.254	11.153	9.245	9.389	-12.012	9.173	8.982	13.461	13.477
1200	-2	9.266	12.045	9.204	13.391	13.487	0.46	13.422	12.632	-6.415	12.617	8.87	6.417	11.163	-10.254	11.153	9.244	9.389	-11.012	9.173	8.982	13.461	13.477
1200	-1	10.628	12.044	9.203	13.39	13.491	1.824	13.426	12.632	-5.413	12.617	8.869	6.416	11.163	-9.254	11.153	9.244	9.388	-10.013	9.172	8.982	13.461	13.477
1200	0	11.778	12.039	9.198	13.382	13.484	2.983	13.419	12.623	0.503	12.608	8.863	6.414	11.154	-8.262	11.144	9.238	9.382	-9.02	9.166	8.975	13.461	13.477
1200	1	12.651	12	9.157	13.322	13.389	3.891	13.321	12.547	6.586	12.532	8.811	6.394	11.091	-7.333	11.081	9.191	9.335	-4.169	9.121	8.924	13.462	13.477
1200	2.301	13.285	11.697	8.851	12.949	12.907	4.584	12.829	12.123	10.424	12.099	8.423	6.122	10.673	-1.951	10.661	8.817	8.959	1.183	8.751	8.539	13.47	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1500	-3	5.354	12.147	9.347	13.402	13.242	-3.476	13.149	12.528	-8.101	12.509	8.995	6.876	11.161	-11.543	11.146	9.404	9.543	-12.001	9.353	9.094	13.456	13.477
1500	-2	7.028	12.147	9.347	13.402	13.243	-1.802	13.149	12.528	-7.1	12.509	8.995	6.876	11.161	-10.543	11.146	9.404	9.543	-11.001	9.353	9.094	13.456	13.477
1500	-1	8.535	12.147	9.347	13.402	13.243	-0.294	13.15	12.528	-6.098	12.509	8.995	6.876	11.161	-9.543	11.146	9.404	9.543	-10.001	9.353	9.094	13.456	13.477
1500	0	9.911	12.147	9.347	13.402	13.246	1.087	13.154	12.529	-2.928	12.51	8.994	6.876	11.161	-8.541	11.146	9.404	9.543	-9.001	9.353	9.093	13.456	13.477
1500	1	11.151	12.144	9.344	13.399	13.252	2.345	13.161	12.528	3.906	12.51	8.991	6.872	11.158	-7.536	11.144	9.4	9.539	-6.736	9.349	9.09	13.458	13.477
1500	2.301	12.51	12.101	9.3	13.352	13.207	3.707	13.117	12.48	9.185	12.461	8.924	6.807	11.098	-3.692	11.081	9.333	9.472	-0.441	9.281	9.023	13.458	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
1800	-3	3.41	12.163	9.401	13.407	13.121	-5.43	13.009	12.478	-8.388	12.457	9.06	7.082	11.161	-11.642	11.142	9.483	9.619	-12.384	9.441	9.146	13.456	13.477
1800	-2	5.124	12.163	9.401	13.407	13.122	-3.717	13.01	12.478	-7.388	12.457	9.06	7.082	11.161	-10.642	11.142	9.483	9.619	-11.384	9.441	9.146	13.456	13.477
1800	-1	6.672	12.163	9.401	13.407	13.122	-2.168	13.01	12.478	-6.387	12.457	9.06	7.082	11.161	-9.642	11.142	9.483	9.619	-10.383	9.441	9.146	13.456	13.477
1800	0	8.099	12.163	9.401	13.407	13.122	-0.738	13.01	12.478	-5.291	12.457	9.06	7.081	11.161	-8.642	11.142	9.483	9.619	-9.383	9.441	9.146	13.456	13.477
1800	1	9.417	12.163	9.401	13.407	13.125	0.59	13.014	12.479	1.119	12.458	9.059	7.08	11.16	-7.641	11.142	9.482	9.618	-8.336	9.44	9.145	13.456	13.477
1800	2.301	11.002	12.156	9.395	13.405	13.139	2.156	13.03	12.483	6.94	12.462	9.044	7.052	11.153	-5.995	11.135	9.464	9.601	-2.53	9.421	9.13	13.456	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
2100	-3	1.867	12.146	9.418	13.41	13.069	-6.976	12.947	12.458	-8.713	12.436	9.095	7.182	11.16	-11.678	11.14	9.521	9.656	-12.008	9.485	9.169	13.456	13.477
2100	-2	3.605	12.146	9.418	13.41	13.069	-5.239	12.947	12.458	-7.713	12.436	9.095	7.182	11.16	-10.678	11.14	9.521	9.656	-11.008	9.485	9.169	13.456	13.477
2100	-1	5.173	12.146	9.418	13.41	13.069	-3.671	12.947	12.458	-6.713	12.436	9.095	7.182	11.16	-9.678	11.14	9.521	9.656	-10.008	9.485	9.169	13.456	13.477
2100	0	6.619	12.146	9.418	13.41	13.069	-2.223	12.947	12.458	-5.712	12.436	9.095	7.182	11.16	-8.678	11.14	9.521	9.656	-9.008	9.485	9.169	13.456	13.477
2100	1	7.955	12.146	9.418	13.41	13.07	-0.881	12.949	12.458	-1.198	12.436	9.095	7.181	11.16	-7.678	11.14	9.52	9.656	-8.008	9.484	9.168	13.456	13.477
2100	2.301	9.574	12.143	9.415	13.41	13.078	0.708	12.957	12.461	4.865	12.439	9.086	7.163	11.156	-6.364	11.137	9.51	9.646	-4.435	9.474	9.16	13.457	13.477

T (K)	log P (atm)	PHOOJ	PH + O2	YOC6JDOA	PHOJ+O	ISOM (2<- 1)	C6JYOO	ISOM (1<- 2)	ISOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM (2<- 3)	ISOM (4<- 3)	Y5JYO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC5OCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward)	Sum (all)
2500	-3	0.284	12.109	9.42	13.413	13.041	-8.545	12.913	12.449	-8.998	12.427	9.123	7.254	11.16	-12.284	11.138	9.547	9.681	-12.707	9.516	9.181	13.458	13.477
2500	-2	2.047	12.109	9.42	13.413	13.041	-6.794	12.913	12.449	-7.998	12.427	9.123	7.254	11.16	-11.284	11.138	9.547	9.681	-11.707	9.516	9.181	13.458	13.477
2500	-1	3.632	12.109	9.42	13.413	13.041	-5.211	12.913	12.449	-6.998	12.427	9.122	7.254	11.16	-10.284	11.138	9.547	9.681	-10.707	9.516	9.181	13.458	13.477
2500	0	5.092	12.109	9.42	13.413	13.041	-3.75	12.913	12.449	-5.998	12.427	9.122	7.254	11.16	-9.283	11.138	9.547	9.681	-9.707	9.516	9.181	13.458	13.477
2500	1	6.443	12.109	9.42	13.413	13.042	-2.396	12.914	12.449	-3.608	12.427	9.122	7.253	11.159	-8.281	11.138	9.546	9.681	-8.706	9.515	9.181	13.458	13.477
2500	2.301	8.077	12.108	9.418	13.413	13.045	-0.8	12.918	12.451	2.663	12.428	9.117	7.241	11.157	-6.941	11.136	9.54	9.674	-6.42	9.509	9.176	13.458	13.477

ChemMaster dissoc output for mac spreadsheet

reactants: PHOOJ

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-03	600	1.667	-6.153	-9.105	-4.495	-3.979	-3.861
1.00E-03	900	1.111	-0.436	-3.295	1.363	1.897	2.01
1.00E-03	1200	0.833	1.503	-1.289	3.402	3.95	4.059
1.00E-03	1500	0.667	2.152	-0.588	4.128	4.687	4.794
1.00E-03	1800	0.556	2.373	-0.325	4.413	4.98	5.085
1.00E-03	2100	0.476	2.45	-0.212	4.544	5.118	5.221
1.00E-03	2500	0.4	2.47	-0.152	4.625	5.208	5.309

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-02	600	1.667	-5.203	-8.155	-3.549	-3.037	-2.918
1.00E-02	900	1.111	0.543	-2.315	2.339	2.871	2.984
1.00E-02	1200	0.833	2.491	-0.3	4.388	4.934	5.044
1.00E-02	1500	0.667	3.144	0.404	5.119	5.676	5.784
1.00E-02	1800	0.556	3.368	0.67	5.407	5.973	6.078
1.00E-02	2100	0.476	3.446	0.784	5.539	6.112	6.216
1.00E-02	2500	0.4	3.468	0.846	5.622	6.204	6.305

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-01	600	1.667	-4.453	-7.406	-2.82	-2.326	-2.202
1.00E-01	900	1.111	1.417	-1.442	3.193	3.708	3.825
1.00E-01	1200	0.833	3.415	0.623	5.295	5.827	5.94
1.00E-01	1500	0.667	4.093	1.352	6.053	6.598	6.708
1.00E-01	1800	0.556	4.33	1.632	6.357	6.913	7.02
1.00E-01	2100	0.476	4.417	1.755	6.5	7.065	7.17
1.00E-01	2500	0.4	4.446	1.824	6.592	7.167	7.27

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E+00	600	1.667	-4.04	-6.999	-2.447	-1.98	-1.849
1.00E+00	900	1.111	2.091	-0.777	3.799	4.267	4.397
1.00E+00	1200	0.833	4.209	1.407	6.015	6.495	6.621
1.00E+00	1500	0.667	4.943	2.193	6.831	7.326	7.448
1.00E+00	1800	0.556	5.211	2.504	7.169	7.677	7.796
1.00E+00	2100	0.476	5.318	2.647	7.337	7.856	7.972
1.00E+00	2500	0.4	5.365	2.735	7.453	7.988	8.1

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E+01	600	1.667	-3.913	-6.874	-2.341	-1.888	-1.754
1.00E+01	900	1.111	2.539	-0.339	4.158	4.565	4.712
1.00E+01	1200	0.833	4.915	2.099	6.585	6.965	7.119
1.00E+01	1500	0.667	5.775	3.01	7.506	7.881	8.036
1.00E+01	1800	0.556	6.106	3.382	7.896	8.274	8.428
1.00E+01	2100	0.476	6.247	3.559	8.092	8.479	8.63
1.00E+01	2500	0.4	7.117	4.463	8.936	9.233	9.413

P (atm)	T (K)	1000/T	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
2.00E+02	600	1.667	-3.892	-6.854	-2.325	-1.874	-1.739
2.00E+02	900	1.111	2.749	-0.134	4.308	4.673	4.832
2.00E+02	1200	0.833	5.601	2.771	7.093	7.32	7.527
2.00E+02	1500	0.667	6.901	4.116	8.372	8.491	8.743
2.00E+02	1800	0.556	7.544	4.798	9.028	9.079	9.362
2.00E+02	2100	0.476	7.907	5.195	9.419	9.43	9.732
2.00E+02	2500	0.4	8.082	5.41	9.644	9.641	9.95

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
600	-3	-6.153	-9.105	-4.495	-3.979	-3.861
600	-2	-5.203	-8.155	-3.549	-3.037	-2.918
600	-1	-4.453	-7.406	-2.82	-2.326	-2.202
600	0	-4.04	-6.999	-2.447	-1.98	-1.849
600	1	-3.913	-6.874	-2.341	-1.888	-1.754
600	2.301	-3.892	-6.854	-2.325	-1.874	-1.739

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
900	-3	-0.436	-3.295	1.363	1.897	2.01
900	-2	0.543	-2.315	2.339	2.871	2.984
900	-1	1.417	-1.442	3.193	3.708	3.825
900	0	2.091	-0.777	3.799	4.267	4.397
900	1	2.539	-0.339	4.158	4.565	4.712
900	2.301	2.749	-0.134	4.308	4.673	4.832

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1200	-3	1.503	-1.289	3.402	3.95	4.059
1200	-2	2.491	-0.3	4.388	4.934	5.044
1200	-1	3.415	0.623	5.295	5.827	5.94
1200	0	4.209	1.407	6.015	6.495	6.621
1200	1	4.915	2.099	6.585	6.965	7.119
1200	2.301	5.601	2.771	7.093	7.32	7.527

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1500	-3	2.152	-0.588	4.128	4.687	4.794
1500	-2	3.144	0.404	5.119	5.676	5.784
1500	-1	4.093	1.352	6.053	6.598	6.708
1500	0	4.943	2.193	6.831	7.326	7.448
1500	1	5.775	3.01	7.506	7.881	8.036
1500	2.301	6.901	4.116	8.372	8.491	8.743

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1800	-3	2.373	-0.325	4.413	4.98	5.085
1800	-2	3.368	0.67	5.407	5.973	6.078
1800	-1	4.33	1.632	6.357	6.913	7.02
1800	0	5.211	2.504	7.169	7.677	7.796
1800	1	6.106	3.382	7.896	8.274	8.428
1800	2.301	7.544	4.798	9.028	9.079	9.362

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
2100	-3	2.45	-0.212	4.544	5.118	5.221
2100	-2	3.446	0.784	5.539	6.112	6.216
2100	-1	4.417	1.755	6.5	7.065	7.17
2100	0	5.318	2.647	7.337	7.856	7.972
2100	1	6.247	3.559	8.092	8.479	8.63
2100	2.301	7.907	5.195	9.419	9.43	9.732

T (K)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
2500	-3	2.47	-0.152	4.625	5.208	5.309
2500	-2	3.468	0.846	5.622	6.204	6.305
2500	-1	4.446	1.824	6.592	7.167	7.27
2500	0	5.365	2.735	7.453	7.988	8.1
2500	1	7.117	4.463	8.936	9.233	9.413
2500	2.301	8.082	5.41	9.644	9.641	9.95

ChemMaster dissoc output for mac spreadsheet

reactants: C6JYOO

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
1.00E-03	600	1.667	-3.973	-4.591	-3.879
1.00E-03	900	1.111	1.952	1.327	2.044
1.00E-03	1200	0.833	3.998	3.368	4.089
1.00E-03	1500	0.667	4.717	4.084	4.808
1.00E-03	1800	0.556	5.001	4.366	5.092
1.00E-03	2100	0.476	5.134	4.496	5.224
1.00E-03	2500	0.4	5.22	4.58	5.31

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
1.00E-02	600	1.667	-2.973	-3.591	-2.879
1.00E-02	900	1.111	2.952	2.327	3.044
1.00E-02	1200	0.833	4.998	4.368	5.089
1.00E-02	1500	0.667	5.717	5.084	5.808
1.00E-02	1800	0.556	6.001	5.366	6.092
1.00E-02	2100	0.476	6.134	5.496	6.224
1.00E-02	2500	0.4	6.22	5.58	6.31

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
1.00E-01	600	1.667	-1.973	-2.592	-1.879
1.00E-01	900	1.111	3.952	3.327	4.044
1.00E-01	1200	0.833	5.998	5.368	6.089
1.00E-01	1500	0.667	6.717	6.084	6.808
1.00E-01	1800	0.556	7.001	6.366	7.092
1.00E-01	2100	0.476	7.134	6.496	7.224
1.00E-01	2500	0.4	7.22	6.58	7.31

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
1.00E+00	600	1.667	-0.973	-1.592	-0.88
1.00E+00	900	1.111	4.952	4.327	5.044
1.00E+00	1200	0.833	6.997	6.368	7.089
1.00E+00	1500	0.667	7.717	7.084	7.808
1.00E+00	1800	0.556	8.001	7.365	8.092
1.00E+00	2100	0.476	8.134	7.496	8.224
1.00E+00	2500	0.4	8.22	7.58	8.31

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
1.00E+01	600	1.667	0.022	-0.597	0.115
1.00E+01	900	1.111	5.949	5.324	6.042
1.00E+01	1200	0.833	7.996	7.367	8.088
1.00E+01	1500	0.667	8.716	8.083	8.807
1.00E+01	1800	0.556	9	8.365	9.091
1.00E+01	2100	0.476	9.134	8.496	9.224
1.00E+01	2500	0.4	9.22	8.579	9.309

P (atm)	T (K)	1000/T	PHOOJ	YOC6JDO	QRRK (tot)
2.00E+02	600	1.667	1.238	0.62	1.332
2.00E+02	900	1.111	7.206	6.581	7.298
2.00E+02	1200	0.833	9.268	8.639	9.36
2.00E+02	1500	0.667	9.996	9.364	10.087
2.00E+02	1800	0.556	10.286	9.65	10.376
2.00E+02	2100	0.476	10.422	9.784	10.512
2.00E+02	2500	0.4	10.511	9.87	10.6

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
600	-3	-3.973	-4.591	-3.879
600	-2	-2.973	-3.591	-2.879
600	-1	-1.973	-2.592	-1.879
600	0	-0.973	-1.592	-0.88
600	1	0.022	-0.597	0.115
600	2.301	1.238	0.62	1.332

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
900	-3	1.952	1.327	2.044
900	-2	2.952	2.327	3.044
900	-1	3.952	3.327	4.044
900	0	4.952	4.327	5.044
900	1	5.949	5.324	6.042
900	2.301	7.206	6.581	7.298

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
1200	-3	3.998	3.368	4.089
1200	-2	4.998	4.368	5.089
1200	-1	5.998	5.368	6.089
1200	0	6.997	6.368	7.089
1200	1	7.996	7.367	8.088
1200	2.301	9.268	8.639	9.36

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
1500	-3	4.717	4.084	4.808
1500	-2	5.717	5.084	5.808
1500	-1	6.717	6.084	6.808
1500	0	7.717	7.084	7.808
1500	1	8.716	8.083	8.807
1500	2.301	9.996	9.364	10.087

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
1800	-3	5.001	4.366	5.092
1800	-2	6.001	5.366	6.092
1800	-1	7.001	6.366	7.092
1800	0	8.001	7.365	8.092
1800	1	9	8.365	9.091
1800	2.301	10.286	9.65	10.376

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
2100	-3	5.134	4.496	5.224
2100	-2	6.134	5.496	6.224
2100	-1	7.134	6.496	7.224
2100	0	8.134	7.496	8.224
2100	1	9.134	8.496	9.224
2100	2.301	10.422	9.784	10.512

T (K)	log P (atm)	PHOOJ	YOC6JDO	QRRK (tot)
2500	-3	5.22	4.58	5.31
2500	-2	6.22	5.58	6.31
2500	-1	7.22	6.58	7.31
2500	0	8.22	7.58	8.31
2500	1	9.22	8.579	9.309
2500	2.301	10.511	9.87	10.6

ChemMaster dissoc output for mac spreadsheet

reactants: YOC6JDO

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E-03	600	1.667	2.766	-15.28	-41.936	-4.696	2.766
1.00E-03	900	1.111	4.534	-12.669	-36.122	-2.687	4.534
1.00E-03	1200	0.833	5.196	-11.664	-33.483	-2.011	5.196
1.00E-03	1500	0.667	5.331	-11.4	-32.228	-1.954	5.331
1.00E-03	1800	0.556	5.06	-11.688	-31.851	-2.381	5.06
1.00E-03	2100	0.476	5.103	-11.612	-31.296	-2.421	5.103
1.00E-03	2500	0.4	5.138	-11.561	-30.783	-2.488	5.138

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E-02	600	1.667	3.1	-10.846	-34.987	-2.952	3.1
1.00E-02	900	1.111	5.265	-8.022	-29.973	-0.368	5.265
1.00E-02	1200	0.833	5.924	-7.282	-28.077	0.347	5.924
1.00E-02	1500	0.667	6.126	-7.123	-27.186	0.525	6.126
1.00E-02	1800	0.556	5.798	-7.707	-27.296	0.035	5.798
1.00E-02	2100	0.476	5.846	-7.758	-26.977	0.019	5.846
1.00E-02	2500	0.4	5.887	-7.845	-26.699	-0.025	5.887

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E-01	600	1.667	3.261	-8.159	-26.081	-2.036	3.261
1.00E-01	900	1.111	5.857	-4.47	-21.523	1.247	5.857
1.00E-01	1200	0.833	6.637	-3.497	-20.29	2.155	6.637
1.00E-01	1500	0.667	6.884	-3.269	-19.983	2.406	6.884
1.00E-01	1800	0.556	7.001	-3.203	-19.865	2.507	7.001
1.00E-01	2100	0.476	6.632	-3.859	-20.612	1.986	6.632
1.00E-01	2500	0.4	6.683	-3.937	-20.678	1.982	6.683

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E+00	600	1.667	3.309	-7.022	-19.331	-1.669	3.309
1.00E+00	900	1.111	6.261	-2.3	-13.482	2.355	6.261
1.00E+00	1200	0.833	7.262	-0.884	-11.935	3.607	7.262
1.00E+00	1500	0.667	7.614	-0.425	-11.575	4.024	7.614
1.00E+00	1800	0.556	7.767	-0.263	-11.579	4.185	7.767
1.00E+00	2100	0.476	7.86	-0.194	-11.688	4.267	7.86
1.00E+00	2500	0.4	7.933	-0.179	-11.917	4.311	7.933

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E+01	600	1.667	3.317	-6.698	-16.662	-1.582	3.317
1.00E+01	900	1.111	6.47	-1.074	-8.866	2.977	6.47
1.00E+01	1200	0.833	7.763	0.976	-6.273	4.709	7.763
1.00E+01	1500	0.667	8.268	1.736	-5.385	5.357	8.269
1.00E+01	1800	0.556	8.494	2.053	-5.08	5.63	8.495
1.00E+01	2100	0.476	8.617	2.205	-4.997	5.766	8.618
1.00E+01	2500	0.4	8.701	2.27	-5.071	5.837	8.701

P (atm)	T (K)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
2.00E+02	600	1.667	3.318	-6.644	-16.014	-1.57	3.318
2.00E+02	900	1.111	6.534	-0.575	-6.696	3.205	6.535
2.00E+02	1200	0.833	8.112	2.278	-2.546	5.488	8.113
2.00E+02	1500	0.667	8.921	3.651	-0.656	6.61	8.924
2.00E+02	1800	0.556	9.325	4.308	0.218	7.15	9.328
2.00E+02	2100	0.476	9.542	4.644	0.645	7.427	9.545
2.00E+02	2500	0.4	9.701	4.874	0.907	7.617	9.704

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
600	-3	2.766	-15.28	-41.936	-4.696	2.766
600	-2	3.1	-10.846	-34.987	-2.952	3.1
600	-1	3.261	-8.159	-26.081	-2.036	3.261
600	0	3.309	-7.022	-19.331	-1.669	3.309
600	1	3.317	-6.698	-16.662	-1.582	3.317
600	2.301	3.318	-6.644	-16.014	-1.57	3.318

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
900	-3	4.534	-12.669	-36.122	-2.687	4.534
900	-2	5.265	-8.022	-29.973	-0.368	5.265
900	-1	5.857	-4.47	-21.523	1.247	5.857
900	0	6.261	-2.3	-13.482	2.355	6.261
900	1	6.47	-1.074	-8.866	2.977	6.47
900	2.301	6.534	-0.575	-6.696	3.205	6.535

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1200	-3	5.196	-11.664	-33.483	-2.011	5.196
1200	-2	5.924	-7.282	-28.077	0.347	5.924
1200	-1	6.637	-3.497	-20.29	2.155	6.637
1200	0	7.262	-0.884	-11.935	3.607	7.262
1200	1	7.763	0.976	-6.273	4.709	7.763
1200	2.301	8.112	2.278	-2.546	5.488	8.113

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1500	-3	5.331	-11.4	-32.228	-1.954	5.331
1500	-2	6.126	-7.123	-27.186	0.525	6.126
1500	-1	6.884	-3.269	-19.983	2.406	6.884
1500	0	7.614	-0.425	-11.575	4.024	7.614
1500	1	8.268	1.736	-5.385	5.357	8.269
1500	2.301	8.921	3.651	-0.656	6.61	8.924

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1800	-3	5.06	-11.688	-31.851	-2.381	5.06
1800	-2	5.798	-7.707	-27.296	0.035	5.798
1800	-1	7.001	-3.203	-19.865	2.507	7.001
1800	0	7.767	-0.263	-11.579	4.185	7.767
1800	1	8.494	2.053	-5.08	5.63	8.495
1800	2.301	9.325	4.308	0.218	7.15	9.328

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
2100	-3	5.103	-11.612	-31.296	-2.421	5.103
2100	-2	5.846	-7.758	-26.977	0.019	5.846
2100	-1	6.632	-3.859	-20.612	1.986	6.632
2100	0	7.86	-0.194	-11.688	4.267	7.86
2100	1	8.617	2.205	-4.997	5.766	8.618
2100	2.301	9.542	4.644	0.645	7.427	9.545

T (K)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
2500	-3	5.138	-11.561	-30.783	-2.488	5.138
2500	-2	5.887	-7.845	-26.699	-0.025	5.887
2500	-1	6.683	-3.937	-20.678	1.982	6.683
2500	0	7.933	-0.179	-11.917	4.311	7.933
2500	1	8.701	2.27	-5.071	5.837	8.701
2500	2.301	9.701	4.874	0.907	7.617	9.704

ChemMaster dissoc output for mac spreadsheet

reactants: Y5JYO4DO

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1.00E-03	600	1.667	5.448	-12.924	-12.487	5.448
1.00E-03	900	1.111	5.87	-10.579	-10.144	5.87
1.00E-03	1200	0.833	5.963	-9.503	-9.07	5.963
1.00E-03	1500	0.667	5.986	-8.881	-8.45	5.986
1.00E-03	1800	0.556	5.985	-8.477	-8.048	5.985
1.00E-03	2100	0.476	5.975	-8.195	-7.768	5.975
1.00E-03	2500	0.4	5.957	-7.93	-7.505	5.957

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1.00E-02	600	1.667	6.447	-11.91	-11.473	6.447
1.00E-02	900	1.111	6.869	-9.572	-9.137	6.869
1.00E-02	1200	0.833	6.963	-8.498	-8.065	6.963
1.00E-02	1500	0.667	6.985	-7.878	-7.447	6.985
1.00E-02	1800	0.556	6.985	-7.474	-7.046	6.985
1.00E-02	2100	0.476	6.975	-7.193	-6.766	6.975
1.00E-02	2500	0.4	6.957	-6.929	-6.504	6.957

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1.00E-01	600	1.667	7.44	-10.776	-10.34	7.44
1.00E-01	900	1.111	7.866	-8.501	-8.066	7.866
1.00E-01	1200	0.833	7.961	-7.452	-7.02	7.961
1.00E-01	1500	0.667	7.984	-6.845	-6.414	7.984
1.00E-01	1800	0.556	7.984	-6.449	-6.02	7.984
1.00E-01	2100	0.476	7.975	-6.172	-5.745	7.975
1.00E-01	2500	0.4	7.956	-5.912	-5.487	7.956

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1.00E+00	600	1.667	8.38	-8.768	-8.331	8.38
1.00E+00	900	1.111	8.836	-6.906	-6.472	8.836
1.00E+00	1200	0.833	8.943	-6.046	-5.613	8.943
1.00E+00	1500	0.667	8.971	-5.541	-5.11	8.971
1.00E+00	1800	0.556	8.975	-5.208	-4.78	8.975
1.00E+00	2100	0.476	8.967	-4.974	-4.547	8.967
1.00E+00	2500	0.4	8.951	-4.753	-4.328	8.951

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1.00E+01	600	1.667	9.126	-4.503	-4.067	9.126
1.00E+01	900	1.111	9.676	-3.32	-2.888	9.676
1.00E+01	1200	0.833	9.827	-2.934	-2.505	9.827
1.00E+01	1500	0.667	9.883	-2.766	-2.339	9.883
1.00E+01	1800	0.556	9.904	-2.683	-2.258	9.904
1.00E+01	2100	0.476	9.909	-2.639	-2.215	9.909
1.00E+01	2500	0.4	9.904	-2.611	-2.189	9.904

P (atm)	T (K)	1000/T	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
2.00E+02	600	1.667	9.726	0.582	0.957	9.726
2.00E+02	900	1.111	10.498	2.41	2.762	10.498
2.00E+02	1200	0.833	10.998	3.576	3.916	10.998
2.00E+02	1500	0.667	11.069	3.672	4.013	11.069
2.00E+02	1800	0.556	11.101	3.655	3.999	11.101
2.00E+02	2100	0.476	11.12	3.601	3.947	11.12
2.00E+02	2500	0.4	11.136	3.504	3.854	11.136

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
600	-3	5.448	-12.924	-12.487	5.448
600	-2	6.447	-11.91	-11.473	6.447
600	-1	7.44	-10.776	-10.34	7.44
600	0	8.38	-8.768	-8.331	8.38
600	1	9.126	-4.503	-4.067	9.126
600	2.301	9.726	0.582	0.957	9.726

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
900	-3	5.87	-10.579	-10.144	5.87
900	-2	6.869	-9.572	-9.137	6.869
900	-1	7.866	-8.501	-8.066	7.866
900	0	8.836	-6.906	-6.472	8.836
900	1	9.676	-3.32	-2.888	9.676
900	2.301	10.498	2.41	2.762	10.498

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1200	-3	5.963	-9.503	-9.07	5.963
1200	-2	6.963	-8.498	-8.065	6.963
1200	-1	7.961	-7.452	-7.02	7.961
1200	0	8.943	-6.046	-5.613	8.943
1200	1	9.827	-2.934	-2.505	9.827
1200	2.301	10.998	3.576	3.916	10.998

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1500	-3	5.986	-8.881	-8.45	5.986
1500	-2	6.985	-7.878	-7.447	6.985
1500	-1	7.984	-6.845	-6.414	7.984
1500	0	8.971	-5.541	-5.11	8.971
1500	1	9.883	-2.766	-2.339	9.883
1500	2.301	11.069	3.672	4.013	11.069

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
1800	-3	5.985	-8.477	-8.048	5.985
1800	-2	6.985	-7.474	-7.046	6.985
1800	-1	7.984	-6.449	-6.02	7.984
1800	0	8.975	-5.208	-4.78	8.975
1800	1	9.904	-2.683	-2.258	9.904
1800	2.301	11.101	3.655	3.999	11.101

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
2100	-3	5.975	-8.195	-7.768	5.975
2100	-2	6.975	-7.193	-6.766	6.975
2100	-1	7.975	-6.172	-5.745	7.975
2100	0	8.967	-4.974	-4.547	8.967
2100	1	9.909	-2.639	-2.215	9.909
2100	2.301	11.12	3.601	3.947	11.12

T (K)	log P (atm)	CY5J+CO2	YOC6JDO	YC5OCJDO	QRRK (tot)
2500	-3	5.957	-7.93	-7.505	5.957
2500	-2	6.957	-6.929	-6.504	6.957
2500	-1	7.956	-5.912	-5.487	7.956
2500	0	8.951	-4.753	-4.328	8.951
2500	1	9.904	-2.611	-2.189	9.904
2500	2.301	11.136	3.504	3.854	11.136

ChemMaster dissoc output for mac spreadsheet

reactants: YC5OCJDO

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E-03	600	1.667	2.133	2.821	2.902
1.00E-03	900	1.111	4.172	4.831	4.918
1.00E-03	1200	0.833	4.679	5.317	5.407
1.00E-03	1500	0.667	4.853	5.475	5.568
1.00E-03	1800	0.556	4.929	5.539	5.634
1.00E-03	2100	0.476	4.966	5.565	5.662
1.00E-03	2500	0.4	4.988	5.575	5.675

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E-02	600	1.667	3.132	3.82	3.901
1.00E-02	900	1.111	5.172	5.831	5.917
1.00E-02	1200	0.833	5.679	6.317	6.407
1.00E-02	1500	0.667	5.853	6.475	6.568
1.00E-02	1800	0.556	5.928	6.538	6.634
1.00E-02	2100	0.476	5.966	6.565	6.662
1.00E-02	2500	0.4	5.988	6.575	6.675

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E-01	600	1.667	4.123	4.81	4.892
1.00E-01	900	1.111	6.168	6.826	6.912
1.00E-01	1200	0.833	6.676	7.314	7.404
1.00E-01	1500	0.667	6.851	7.473	7.566
1.00E-01	1800	0.556	6.927	7.536	7.632
1.00E-01	2100	0.476	6.964	7.563	7.661
1.00E-01	2500	0.4	6.987	7.574	7.674

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E+00	600	1.667	5.05	5.73	5.812
1.00E+00	900	1.111	7.129	7.78	7.868
1.00E+00	1200	0.833	7.651	8.283	8.374
1.00E+00	1500	0.667	7.832	8.449	8.543
1.00E+00	1800	0.556	7.913	8.518	8.614
1.00E+00	2100	0.476	7.953	8.548	8.646
1.00E+00	2500	0.4	7.978	8.561	8.662

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E+01	600	1.667	5.741	6.392	6.479
1.00E+01	900	1.111	7.944	8.562	8.656
1.00E+01	1200	0.833	8.517	9.114	9.212
1.00E+01	1500	0.667	8.726	9.31	9.411
1.00E+01	1800	0.556	9.845	10.335	10.457
1.00E+01	2100	0.476	9.881	10.365	10.488
1.00E+01	2500	0.4	9.908	10.386	10.511

P (atm)	T (K)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
2.00E+02	600	1.667	6.128	6.743	6.837
2.00E+02	900	1.111	8.673	9.2	9.313
2.00E+02	1200	0.833	9.412	9.874	10.003
2.00E+02	1500	0.667	10.03	10.377	10.538
2.00E+02	1800	0.556	10.241	10.541	10.717
2.00E+02	2100	0.476	10.297	10.581	10.763
2.00E+02	2500	0.4	10.336	10.609	10.795

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
600	-3	2.133	2.821	2.902
600	-2	3.132	3.82	3.901
600	-1	4.123	4.81	4.892
600	0	5.05	5.73	5.812
600	1	5.741	6.392	6.479
600	2.301	6.128	6.743	6.837

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
900	-3	4.172	4.831	4.918
900	-2	5.172	5.831	5.917
900	-1	6.168	6.826	6.912
900	0	7.129	7.78	7.868
900	1	7.944	8.562	8.656
900	2.301	8.673	9.2	9.313

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1200	-3	4.679	5.317	5.407
1200	-2	5.679	6.317	6.407
1200	-1	6.676	7.314	7.404
1200	0	7.651	8.283	8.374
1200	1	8.517	9.114	9.212
1200	2.301	9.412	9.874	10.003

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1500	-3	4.853	5.475	5.568
1500	-2	5.853	6.475	6.568
1500	-1	6.851	7.473	7.566
1500	0	7.832	8.449	8.543
1500	1	8.726	9.31	9.411
1500	2.301	10.03	10.377	10.538

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1800	-3	4.929	5.539	5.634
1800	-2	5.928	6.538	6.634
1800	-1	6.927	7.536	7.632
1800	0	7.913	8.518	8.614
1800	1	9.845	10.335	10.457
1800	2.301	10.241	10.541	10.717

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
2100	-3	4.966	5.565	5.662
2100	-2	5.966	6.565	6.662
2100	-1	6.964	7.563	7.661
2100	0	7.953	8.548	8.646
2100	1	9.881	10.365	10.488
2100	2.301	10.297	10.581	10.763

T (K)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
2500	-3	4.988	5.575	5.675
2500	-2	5.988	6.575	6.675
2500	-1	6.987	7.574	7.674
2500	0	7.978	8.561	8.662
2500	1	9.908	10.386	10.511
2500	2.301	10.336	10.609	10.795

Modified Arrhenius fits of the rate constants for the product channels of phenyl + O2 and its stable products

Mar 2001 (chemast) PH + O2 => Products low for sensitivity Low jwb / N sebar

PH + O2	<=> PHOOJ	1.03+107	-30.86	24144.	!	1.00E-03 atm,	600-2500 K,	44% err	::CM	:
PH + O2	<=> PHOOJ	6.34+114	-32.44	31730.	!	1.00E-02 atm,	600-2500 K,	45% err	::CM	:
PH + O2	<=> PHOOJ	4.75+122	-34.07	40095.	!	1.00E-01 atm,	600-2500 K,	41% err	::CM	:
PH + O2	<=> PHOOJ	8.76+127	-34.99	47402.	!	1.00E+00 atm,	600-2500 K,	32% err	::CM	:
PH + O2	<=> PHOOJ	3.23+127	-34.33	51398.	!	1.00E+01 atm,	600-2500 K,	42% err	::CM	:
PH + O2	<=> PHOOJ	1.31+116	-30.47	49865.	!	2.00E+02 atm,	600-2500 K,	83% err	::CM	:
PH + O2	<=> PH + O2	1.08E+19	-1.85	7075.	!	1.00E-03 atm,	600-2500 K,	3% err	::CM	:
PH + O2	<=> PH + O2	1.19E+20	-2.14	7947.	!	1.00E-02 atm,	600-2500 K,	2% err	::CM	:
PH + O2	<=> PH + O2	5.86E+23	-3.15	11064.	!	1.00E-01 atm,	600-2500 K,	2% err	::CM	:
PH + O2	<=> PH + O2	1.18E+31	-5.15	17472.	!	1.00E+00 atm,	600-2500 K,	9% err	::CM	:
PH + O2	<=> PH + O2	1.17E+39	-7.30	25376.	!	1.00E+01 atm,	600-2500 K,	11% err	::CM	:
PH + O2	<=> PH + O2	3.44E+41	-7.84	31725.	!	2.00E+02 atm,	600-2500 K,	16% err	::CM	:
PH + O2	<=> YOC6JDOA	1.94E+14	-1.26	6662.	!	1.00E-03 atm,	600-2500 K,	3% err	::CM	:
PH + O2	<=> YOC6JDOA	2.42E+15	-1.56	7577.	!	1.00E-02 atm,	600-2500 K,	2% err	::CM	:
PH + O2	<=> YOC6JDOA	1.49E+19	-2.60	10779.	!	1.00E-01 atm,	600-2500 K,	3% err	::CM	:
PH + O2	<=> YOC6JDOA	3.49E+26	-4.61	17253.	!	1.00E+00 atm,	600-2500 K,	9% err	::CM	:
PH + O2	<=> YOC6JDOA	3.17E+34	-6.75	25151.	!	1.00E+01 atm,	600-2500 K,	11% err	::CM	:
PH + O2	<=> YOC6JDOA	6.95E+36	-7.26	31429.	!	2.00E+02 atm,	600-2500 K,	16% err	::CM	:
PH + O2	<=> PHOJ+O	4.09E+14	-0.32	1248.	!	1.00E-03 atm,	600-2500 K,	1% err	::CM	:
PH + O2	<=> PHOJ+O	4.22E+16	-0.87	2930.	!	1.00E-02 atm,	600-2500 K,	3% err	::CM	:
PH + O2	<=> PHOJ+O	6.21E+21	-2.29	7327.	!	1.00E-01 atm,	600-2500 K,	9% err	::CM	:
PH + O2	<=> PHOJ+O	7.06E+29	-4.49	14560.	!	1.00E+00 atm,	600-2500 K,	15% err	::CM	:
PH + O2	<=> PHOJ+O	1.40E+37	-6.44	22258.	!	1.00E+01 atm,	600-2500 K,	15% err	::CM	:
PH + O2	<=> PHOJ+O	4.29E+37	-6.42	27510.	!	2.00E+02 atm,	600-2500 K,	17% err	::CM	:
PH + O2	<=> C6JYOO	2.83E+94	-29.85	20653.	!	1.00E-03 atm,	600-2500 K,	42% err	::CM	:
PH + O2	<=> C6JYOO	2.80+102	-31.49	28348.	!	1.00E-02 atm,	600-2500 K,	42% err	::CM	:
PH + O2	<=> C6JYOO	1.90+110	-33.11	36654.	!	1.00E-01 atm,	600-2500 K,	38% err	::CM	:
PH + O2	<=> C6JYOO	1.08+115	-33.89	43428.	!	1.00E+00 atm,	600-2500 K,	32% err	::CM	:
PH + O2	<=> C6JYOO	1.20+113	-32.82	45766.	!	1.00E+01 atm,	600-2500 K,	45% err	::CM	:
PH + O2	<=> C6JYOO	3.44E+94	-27.05	37025.	!	2.00E+02 atm,	600-2500 K,	101% err	::CM	:
PH + O2	<=> YOC6JDO	5.69E+11	-6.02	4132.	!	1.00E-03 atm,	600-2500 K,	16% err	::CM	:
PH + O2	<=> YOC6JDO	2.33E+16	-7.01	7127.	!	1.00E-02 atm,	600-2500 K,	20% err	::CM	:
PH + O2	<=> YOC6JDO	8.07E-32	6.24	-35021.	!	1.00E-01 atm,	600-2500 K,	39% err	::CM	:
PH + O2	<=> YOC6JDO	4.45E+68	-22.25	1519.	!	1.00E+00 atm,	600-2500 K,	698% err	::CM	:
PH + O2	<=> YOC6JDO	4.16+183	-53.27	73051.	!	1.00E+01 atm,	600-2500 K,	59% err	::CM	:
PH + O2	<=> YOC6JDO	1.15+181	-50.16	89761.	!	2.00E+02 atm,	600-2500 K,	113% err	::CM	:
PH + O2	<=> RODC6JDO	6.62E+12	-0.17	-1677.	!	1.00E-03 atm,	600-2500 K,	5% err	::CM	:
PH + O2	<=> RODC6JDO	3.70E+15	-0.92	615.	!	1.00E-02 atm,	600-2500 K,	8% err	::CM	:
PH + O2	<=> RODC6JDO	4.19E+21	-2.58	5787.	!	1.00E-01 atm,	600-2500 K,	15% err	::CM	:
PH + O2	<=> RODC6JDO	9.46E+29	-4.85	13401.	!	1.00E+00 atm,	600-2500 K,	21% err	::CM	:
PH + O2	<=> RODC6JDO	7.47E+36	-6.69	21002.	!	1.00E+01 atm,	600-2500 K,	18% err	::CM	:
PH + O2	<=> RODC6JDO	1.68E+43	-8.25	31871.	!	2.00E+02 atm,	600-2500 K,	16% err	::CM	:
PH + O2	<=> YOC5J+CO	6.35E+07	0.43	1455.	!	1.00E-03 atm,	600-2500 K,	5% err	::CM	:
PH + O2	<=> YOC5J+CO	7.63E+09	-0.14	3189.	!	1.00E-02 atm,	600-2500 K,	2% err	::CM	:
PH + O2	<=> YOC5J+CO	1.23E+15	-1.57	7600.	!	1.00E-01 atm,	600-2500 K,	4% err	::CM	:
PH + O2	<=> YOC5J+CO	2.17E+23	-3.82	14920.	!	1.00E+00 atm,	600-2500 K,	10% err	::CM	:
PH + O2	<=> YOC5J+CO	1.09E+32	-6.16	23658.	!	1.00E+01 atm,	600-2500 K,	12% err	::CM	:
PH + O2	<=> YOC5J+CO	2.77E+40	-8.29	36087.	!	2.00E+02 atm,	600-2500 K,	15% err	::CM	:
PH + O2	<=> Y5JYO4DO	1.19E+04	-4.66	4723.	!	1.00E-03 atm,	600-2500 K,	31% err	::CM	:

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PH + O2          <=> Y5JYO4DO      6.97E+07   -5.42    7027.   ! 1.00E-02 atm,  600-2500 K,  33% err  ::CM  :
PH + O2          <=> Y5JYO4DO      2.57E+14   -6.95   11778.   ! 1.00E-01 atm,  600-2500 K,  37% err  ::CM  :
PH + O2          <=> Y5JYO4DO      3.60E+23   -9.16   19178.   ! 1.00E+00 atm,  600-2500 K,  39% err  ::CM  :
PH + O2          <=> Y5JYO4DO      3.07E-10    0.26   -7306.   ! 1.00E+01 atm,  600-2500 K,  54% err  ::CM  :
PH + O2          <=> Y5JYO4DO      1.72E+72  -22.87   23182.   ! 2.00E+02 atm,  600-2500 K, 202% err  ::CM  :
PH + O2          <=> CY5J+CO2      9.48E+10    0.04    -292.   ! 1.00E-03 atm,  600-2500 K,   0% err  ::CM  :
PH + O2          <=> CY5J+CO2      2.48E+13   -0.62    1725.   ! 1.00E-02 atm,  600-2500 K,   3% err  ::CM  :
PH + O2          <=> CY5J+CO2      1.11E+19   -2.17    6533.   ! 1.00E-01 atm,  600-2500 K,   9% err  ::CM  :
PH + O2          <=> CY5J+CO2      2.40E+27   -4.44   14029.   ! 1.00E+00 atm,  600-2500 K,  15% err  ::CM  :
PH + O2          <=> CY5J+CO2      1.93E+35   -6.56   22297.   ! 1.00E+01 atm,  600-2500 K,  15% err  ::CM  :
PH + O2          <=> CY5J+CO2      3.40E+42   -8.37   33939.   ! 2.00E+02 atm,  600-2500 K,  15% err  ::CM  :
PH + O2          <=> YC5OCJDO      2.36E-02   -3.13    3144.   ! 1.00E-03 atm,  600-2500 K,  45% err  ::CM  :
PH + O2          <=> YC5OCJDO      1.21E+02   -3.88    5402.   ! 1.00E-02 atm,  600-2500 K,  46% err  ::CM  :
PH + O2          <=> YC5OCJDO      4.64E+08   -5.41   10138.   ! 1.00E-01 atm,  600-2500 K,  50% err  ::CM  :
PH + O2          <=> YC5OCJDO      7.12E-48   10.12  -39445.   ! 1.00E+00 atm,  600-2500 K,  78% err  ::CM  :
PH + O2          <=> YC5OCJDO      1.86E+27  -11.05  -11715.   ! 1.00E+01 atm,  600-2500 K, 330% err  ::CM  :
PH + O2          <=> YC5OCJDO      1.53+140  -41.66   58316.   ! 2.00E+02 atm,  600-2500 K,  20% err  ::CM  :
PH + O2          <=> CY5J+CO2      3.77E+08    0.36    2788.   ! 1.00E-03 atm,  600-2500 K,   7% err  ::CM  :
PH + O2          <=> CY5J+CO2      2.80E+10   -0.15    4347.   ! 1.00E-02 atm,  600-2500 K,   5% err  ::CM  :
PH + O2          <=> CY5J+CO2      2.24E+15   -1.50    8492.   ! 1.00E-01 atm,  600-2500 K,   1% err  ::CM  :
PH + O2          <=> CY5J+CO2      3.07E+23   -3.72   15664.   ! 1.00E+00 atm,  600-2500 K,   8% err  ::CM  :
PH + O2          <=> CY5J+CO2      3.64E+32   -6.17   24604.   ! 1.00E+01 atm,  600-2500 K,  10% err  ::CM  :
PH + O2          <=> CY5J+CO2      1.48E+42   -8.64   37911.   ! 2.00E+02 atm,  600-2500 K,  15% err  ::CM  :
PHOOJ      <=> PH + O2         4.31E+72  -18.83   72448.   ! 1.00E-03 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PH + O2         8.10E+73  -18.91   72779.   ! 1.00E-02 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PH + O2         5.96E+75  -19.14   74104.   ! 1.00E-01 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PH + O2         2.60E+78  -19.57   76898.   ! 1.00E+00 atm,  600-2500 K,  32% err  ::CM  :
PHOOJ      <=> PH + O2         6.81E+65  -15.55   72524.   ! 1.00E+01 atm,  600-2500 K,  88% err  ::CM  :
PHOOJ      <=> PH + O2         1.40E+65  -14.83   76396.   ! 2.00E+02 atm,  600-2500 K,   5% err  ::CM  :
PHOOJ      <=> YOC6JDOA        1.60E+68  -18.30   72453.   ! 1.00E-03 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> YOC6JDOA        2.99E+69  -18.38   72781.   ! 1.00E-02 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> YOC6JDOA        2.13E+71  -18.60   74100.   ! 1.00E-01 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> YOC6JDOA        7.31E+73  -19.01   76826.   ! 1.00E+00 atm,  600-2500 K,  32% err  ::CM  :
PHOOJ      <=> YOC6JDOA        2.29E+61  -15.02   72449.   ! 1.00E+01 atm,  600-2500 K,  88% err  ::CM  :
PHOOJ      <=> YOC6JDOA        4.19E+60  -14.29   76223.   ! 2.00E+02 atm,  600-2500 K,   5% err  ::CM  :
PHOOJ      <=> PHOJ+O          1.13E+72  -18.03   72444.   ! 1.00E-03 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PHOJ+O          2.08E+73  -18.10   72778.   ! 1.00E-02 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PHOJ+O          1.04E+75  -18.28   74050.   ! 1.00E-01 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PHOJ+O          6.97E+76  -18.51   76313.   ! 1.00E+00 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> PHOJ+O          2.52E+65  -14.89   72080.   ! 1.00E+01 atm,  600-2500 K,  80% err  ::CM  :
PHOOJ      <=> PHOJ+O          5.94E+64  -14.31   75041.   ! 2.00E+02 atm,  600-2500 K,   8% err  ::CM  :
PHOOJ      <=> C6JYOO          1.78E+72  -17.92   72431.   ! 1.00E-03 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> C6JYOO          3.25E+73  -17.99   72775.   ! 1.00E-02 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> C6JYOO          1.19E+75  -18.13   74007.   ! 1.00E-01 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> C6JYOO          2.26E+76  -18.22   75906.   ! 1.00E+00 atm,  600-2500 K,  31% err  ::CM  :
PHOOJ      <=> C6JYOO          2.83E+66  -15.10   72138.   ! 1.00E+01 atm,  600-2500 K,  72% err  ::CM  :
PHOOJ      <=> C6JYOO          3.13E+67  -15.12   75039.   ! 2.00E+02 atm,  600-2500 K,  14% err  ::CM  :
C6JYOO     <=> PHOOJ           3.80E+73  -18.29   73232.   ! 1.00E-03 atm,  600-2500 K,  33% err  ::CM  :
C6JYOO     <=> PHOOJ           3.80E+74  -18.29   73232.   ! 1.00E-02 atm,  600-2500 K,  33% err  ::CM  :
C6JYOO     <=> PHOOJ           3.80E+75  -18.29   73232.   ! 1.00E-01 atm,  600-2500 K,  33% err  ::CM  :
C6JYOO     <=> PHOOJ           3.82E+76  -18.29   73235.   ! 1.00E+00 atm,  600-2500 K,  33% err  ::CM  :
C6JYOO     <=> PHOOJ           3.99E+77  -18.29   73262.   ! 1.00E+01 atm,  600-2500 K,  33% err  ::CM  :
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C6JYOO	<=>	PHOOJ	1.45E+79	-18.36	73681.	!	2.00E+02 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	1.15E+73	-18.32	73232.	!	1.00E-03 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	1.15E+74	-18.32	73232.	!	1.00E-02 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	1.15E+75	-18.32	73232.	!	1.00E-01 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	1.15E+76	-18.32	73235.	!	1.00E+00 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	1.20E+77	-18.33	73261.	!	1.00E+01 atm,	600-2500 K,	33% err	::CM	:
C6JYOO	<=>	YOC6JDO	4.41E+78	-18.40	73683.	!	2.00E+02 atm,	600-2500 K,	33% err	::CM	:
YOC6JDO	<=>	RODC6JDO	3.44E+34	-8.02	25970.	!	1.00E-03 atm,	600-2500 K,	23% err	::CM	:
YOC6JDO	<=>	RODC6JDO	1.56E+41	-9.65	30900.	!	1.00E-02 atm,	600-2500 K,	29% err	::CM	:
YOC6JDO	<=>	RODC6JDO	8.44E+47	-11.22	37021.	!	1.00E-01 atm,	600-2500 K,	18% err	::CM	:
YOC6JDO	<=>	RODC6JDO	3.42E+40	-8.71	35665.	!	1.00E+00 atm,	600-2500 K,	18% err	::CM	:
YOC6JDO	<=>	RODC6JDO	1.41E+40	-8.30	37791.	!	1.00E+01 atm,	600-2500 K,	8% err	::CM	:
YOC6JDO	<=>	RODC6JDO	7.25E+30	-5.31	35175.	!	2.00E+02 atm,	600-2500 K,	9% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	1.67E+28	-10.81	36951.	!	1.00E-03 atm,	600-2500 K,	29% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	2.55E+48	-15.48	44477.	!	1.00E-02 atm,	600-2500 K,	42% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	2.96E+64	-18.72	56526.	!	1.00E-01 atm,	600-2500 K,	29% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	5.96E+58	-15.88	59310.	!	1.00E+00 atm,	600-2500 K,	34% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	9.01E+64	-16.71	69146.	!	1.00E+01 atm,	600-2500 K,	23% err	::CM	:
YOC6JDO	<=>	YOC5J+CO	1.30E+52	-12.12	68985.	!	2.00E+02 atm,	600-2500 K,	14% err	::CM	:
YOC6JDO	<=>	C6JYOO	2.84E+09	-10.28	62648.	!	1.00E-03 atm,	600-2500 K,	29% err	::CM	:
YOC6JDO	<=>	C6JYOO	6.11E+26	-14.24	60827.	!	1.00E-02 atm,	600-2500 K,	43% err	::CM	:
YOC6JDO	<=>	C6JYOO	3.72E+60	-22.20	68439.	!	1.00E-01 atm,	600-2500 K,	36% err	::CM	:
YOC6JDO	<=>	C6JYOO	4.38E+77	-24.36	80121.	!	1.00E+00 atm,	600-2500 K,	46% err	::CM	:
YOC6JDO	<=>	C6JYOO	7.44E+92	-26.31	99751.	!	1.00E+01 atm,	600-2500 K,	38% err	::CM	:
YOC6JDO	<=>	C6JYOO	6.48E+82	-21.31	108893.	!	2.00E+02 atm,	600-2500 K,	14% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	9.35E+38	-11.40	32843.	!	1.00E-03 atm,	600-2500 K,	28% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	4.19E+48	-13.36	39573.	!	1.00E-02 atm,	600-2500 K,	37% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	3.54E+58	-15.44	48491.	!	1.00E-01 atm,	600-2500 K,	25% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	3.90E+52	-12.97	49842.	!	1.00E+00 atm,	600-2500 K,	28% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	2.25E+55	-13.16	55805.	!	1.00E+01 atm,	600-2500 K,	16% err	::CM	:
YOC6JDO	<=>	Y5JYO4DO	1.88E+43	-9.10	53818.	!	2.00E+02 atm,	600-2500 K,	12% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	3.20E+12	-1.78	5733.	!	1.00E-03 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	3.23E+13	-1.79	5738.	!	1.00E-02 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	3.49E+14	-1.79	5782.	!	1.00E-01 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	5.78E+15	-1.85	6104.	!	1.00E+00 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	7.65E+16	-1.88	6917.	!	1.00E+01 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	CY5J+CO2	5.84E+20	-2.56	10845.	!	2.00E+02 atm,	600-2500 K,	8% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	3.28E-02	-1.36	20997.	!	1.00E-03 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	2.95E-01	-1.35	20926.	!	1.00E-02 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	1.14E+00	-1.24	20264.	!	1.00E-01 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	3.08E-01	-0.83	16299.	!	1.00E+00 atm,	600-2500 K,	2% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	2.73E+09	-3.20	13817.	!	1.00E+01 atm,	600-2500 K,	6% err	::CM	:
Y5JYO4DO	<=>	YOC6JDO	2.48E+34	-8.34	29394.	!	2.00E+02 atm,	600-2500 K,	24% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	1.18E-01	-1.40	21039.	!	1.00E-03 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	1.06E+00	-1.39	20968.	!	1.00E-02 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	4.09E+00	-1.28	20305.	!	1.00E-01 atm,	600-2500 K,	3% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	1.10E+00	-0.87	16338.	!	1.00E+00 atm,	600-2500 K,	2% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	8.90E+09	-3.23	13824.	!	1.00E+01 atm,	600-2500 K,	6% err	::CM	:
Y5JYO4DO	<=>	YC5OCJDO	1.51E+34	-8.18	28955.	!	2.00E+02 atm,	600-2500 K,	23% err	::CM	:
YC5OCJDO	<=>	CY5J+CO2	8.91E+29	-6.74	24845.	!	1.00E-03 atm,	600-2500 K,	18% err	::CM	:
YC5OCJDO	<=>	CY5J+CO2	8.99E+30	-6.74	24850.	!	1.00E-02 atm,	600-2500 K,	18% err	::CM	:
YC5OCJDO	<=>	CY5J+CO2	9.72E+31	-6.75	24899.	!	1.00E-01 atm,	600-2500 K,	18% err	::CM	:

YC5OCJDO	<=> CY5J+CO2	1.61E+33	-6.80	25257.	!	1.00E+00 atm,	600-2500 K,	19% err	::CM	:
YC5OCJDO	<=> CY5J+CO2	1.02E+13	-0.47	16211.	!	1.00E+01 atm,	600-2500 K,	66% err	::CM	:
YC5OCJDO	<=> CY5J+CO2	2.45E+33	-6.05	28628.	!	2.00E+02 atm,	600-2500 K,	13% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	1.15E+31	-6.89	24827.	!	1.00E-03 atm,	600-2500 K,	18% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	1.16E+32	-6.89	24832.	!	1.00E-02 atm,	600-2500 K,	18% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	1.25E+33	-6.90	24882.	!	1.00E-01 atm,	600-2500 K,	19% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	1.90E+34	-6.95	25234.	!	1.00E+00 atm,	600-2500 K,	19% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	3.47E+15	-1.06	16853.	!	1.00E+01 atm,	600-2500 K,	59% err	::CM	:
YC5OCJDO	<=> Y5JYO4DO	2.67E+35	-6.58	28453.	!	2.00E+02 atm,	600-2500 K,	12% err	::CM	: