Preprint UCRL-JC-142418

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This article was submitted to 2nd Joint Meeting of the US Sections of the Combustion Institute, Oakland, CA., March 25-28, 2001

U.S. Department of Energy



April 12, 2001

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Reaction of Phenyl Radical with O₂: Thermodynamic Properties, Important Reaction Paths and Kinetics

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Presented at the 2nd Joint Meeting of the US Sections of the Combustion Institute March 25-28, 2001 Oakland, California Paper 99

Reaction of Phenyl Radical with O_2 : Thermodynamic Properties, Important Reaction Paths and Kinetics

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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 (S₂₉₈), 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 benzene¹⁻⁶, toluene^{7,8 and} phenol⁹ 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 Mackie¹¹ and Louw¹² research groups has also shown that phenoxy radical is an important intermediate in pyrolysis and oxidation of an isole 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 \rightarrow 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:

 $C6 \Rightarrow$ (phenoxy) -> C5 (cyclopentadienyl) -->(+O₂) => O + Cyclic C₅H₅O.

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

Wang and Brezinsky¹⁸ 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 al¹. 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 NO₂ addition. The benzene oxidation rate doubled in the presence of NO₂ 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. Bittker¹⁹ 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 Frank²¹ 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 al⁴ 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 al² 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 Skevis³ 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 Carpenter²⁵, 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 calculations²⁷⁻³⁰. 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 ($\Delta H^{o}_{f(298)}$), Entropy S₂₉₈, 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 + O₂ calculation data of Mebel et al, and phenyl + O₂ 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, $H_{f}^{\circ}_{(298)}$, $S_{f}^{\circ}_{(298)}$, 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 al³⁴, Eqn. 4.7.
- d. The Leonard-Jones collision frequency Z_{LJ} is now calculated by $Z_{LJ} = Z \Omega$ integral³⁵⁻³⁷ obtained from fit of Reid et al³⁷.

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 al³⁹, Bozzelli et al⁴⁰⁻⁴². 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 systems⁴⁹. 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 + O₂ 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 $\Delta H_{f^{2}298}^{\circ}$, 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 $\Delta H_{f 298}^{e}$ values for small (C₁ to C₃) molecules.^{b26}

Thermodynamic Properties Using ab initio Calculations

Enthalpy, $\Delta H_{f~298}^{o}$, entropy, S_{298}^{o} 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 ($\Delta H_r^{\circ}_{298}$) 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 \bullet 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 Tⁿ 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 CO₂ + 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 estimated²⁸⁻³⁰.

Results and Discussion - Chemical Activation Reaction – Phenyl + O2

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 C₅H₅O radical (O=C-C=C-C=C-O). 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 CO₂. For dissociation of this phenylperoxy adduct two channels are competitive:

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

Acknowledgments

The work at LLNL was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48 and supported by the US Department of Energy, Office of Transportation Technologies, Steve Chalk and Gurpreet Singh, program managers, and by the Office of Basic Energy Sciences, Division of Chemical Sciences, William Kirchhoff, program manager.

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

PHOOH + CH_3 - $CH_3 \Rightarrow Ph + CH_3$ - CH_2OOH	PHOOH = -3.377
$\mathbf{PHOOH} + \mathbf{CH}_2 = \mathbf{CH}_2 => \mathbf{Ph} + \mathbf{CH}_2 = \mathbf{CHOOH}$	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 ₂ OOH	PHCOOH = -8.13
PHCOOH + CH ₂ =CH-CH ₃ => Toluene + CH ₂ =CH-CH ₂ OOH	PHCOOH = -7.19 Average = -8.02
PHCOO . + $CH_3OOH => PHCOOH + CH_3OO$.	PHCOO. = 29.81



Fig. 2





cdco-o

Fig. 3





Fig. 5 (Mar 2001 (chemast) $PH + O_2 => Products$





Fig. 6: Dissociation for PHOOJ

Appendix

reactant	s: PH + O2																							
P (atm) 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0:	T (K) 3 60 3 90 3 120 3 150 3 180 3 180 3 210 3 250	1000/T 30 1 30 0 30 0 30 0 30 0 30 0 30 0	PHOCJ 667 12.394 111 10.187 833 7.694 867 5.354 556 3.44 556 3.44 1476 1.865 0.4 0.284	PH + O2 11.325 11.815 12.045 12.147 12.163 12.146 12.109	YOC6JDOA 8,38 8,927 9,204 9,347 9,401 9,418 9,42	PHOJ+O 13.259 13.366 13.391 13.402 13.407 13.41 13.413	SOM (2<- 1) Cl 14.324 13.851 13.496 13.242 13.121 13.069 13.041	50YOO IS 3.923 1.435 -1.107 -3.476 -5.43 -6.976 -8.545	SOM (1<-2) IS 14.305 13.812 13.42 13.149 13.009 12.947 12.913	COM (3<-2)Y(12.961 12.784 12.632 12.528 12.478 12.478 12.458 12.449	DC6JD0 -6.501 -7.02 -7.415 -8.101 -8.388 -8.713 -8.998	RODC6JDO 12.954 12.773 12.617 12.509 12.457 12.436 12.427	(OC5J+CO IS 8.492 8.689 8.87 8.995 9.06 9.095 9.123	OM (2<-3) 4.401 5.581 6.417 6.876 7.082 7.182 7.254	SOM (4~ 3) 11.197 11.171 11.163 11.163 11.161 11.16 11.16	Y5,YO4DO -10.624 -10.684 -11.254 -11.543 -11.642 -11.678 -12.284	CY5J+CO2 11.194 11.166 11.153 11.146 11.142 11.14 11.138	ISOM (3<-4) 8.743 9.007 9.245 9.404 9.483 9.521 9.547	ISOM (5<-4) 8.907 9.16 9.389 9.543 9.619 9.656 9.681	/C50CJD0 0 -11.5 -11.522 -12.012 -12.001 -12.384 -12.008 -12.707	Y5J+CO2 IS 8.582 8.899 9.173 9.353 9.441 9.485 9.516	OM (4<-5) S 8.629 8.815 8.982 9.094 9.146 9.169 9.181	um (forward) S 13.474 13.468 13.461 13.456 13.456 13.456 13.456 13.458	um (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
P (atm) 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0: 1.00E-0:	T (K) 2 60 2 90 2 120 2 150 2 150 2 180 2 210 2 250	1000/T 30 1 30 1 30 0 30 0 30 0 30 0 30 0	PHOOJ .667 13.039 .111 11.434 .833 9.266 .667 7.024 .556 5.124 .476 3.600 0.4 2.04	PH + O2 11.25 11.813 12.045 12.147 12.163 12.146 12.109	YOO6JDOA 8.302 8.925 9.204 9.347 9.401 9.418 9.42	PHOJ+O I 13.115 13.363 13.391 13.402 13.407 13.41 13.413	SOM (2<- 1) C/ 14.079 13.849 13.487 13.243 13.122 13.069 13.041	6JYOO 15 4.565 2.688 0.46 -1.802 -3.717 -5.239 -6.794	SOM (1<-2) IS 14.057 13.811 13.422 13.149 13.01 12.947 12.913	COM (3<- 2) YG 12.767 12.779 12.632 12.528 12.478 12.458 12.458 12.449	OC6JDO 1 -5.753 -6.021 -6.415 -7.1 -7.388 -7.713 -7.998	RODC8JDO 12.759 12.769 12.617 12.509 12.457 12.436 12.427	(OC5.#CO (S 8.344 8.686 8.87 8.995 9.06 9.095 9.123	OM (2<-3) 4.349 5.58 6.417 6.876 7.082 7.182 7.254	ISOM (4<-3) 11.026 11.167 11.163 11.161 11.161 11.16 11.16	Y5JYO4DO -9.819 -9.687 -10.254 -10.543 -10.642 -10.678 -11.284	CY5J+CO2 11.023 11.162 11.153 11.146 11.142 11.14 11.138	ISOM (3<- 4) 8.605 9.004 9.244 9.404 9.483 9.521 9.521 9.547	ISOM (5<- 4) 8.768 9.157 9.389 9.543 9.643 9.656 9.661	YC50CJD0 0 -10.692 -10.526 -11.012 -11.001 -11.384 -11.008 -11.707	2Y5J+CO2 IS 8,449 8,896 9,173 9,353 9,441 9,485 9,516	CM (4<-5) S 8.484 8.812 8.982 9.094 9.146 9.169 9.181	ium (forward) S 13.475 13.468 13.461 13.456 13.456 13.456 13.456 13.456	Sum (ali) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
P (atm) 1.00E-0 1.00E-0 1.00E-0 1.00E-0 1.00E-0 1.00E-0 1.00E-0	T (K) 1 60 1 90 1 120 1 120 1 120 1 210 1 250	1000/7 20 1 20 1 20 0 20 0 20 0 20 0 20 0	PHOOJ .667 13.355 .111 12.384 .667 8.533 .556 6.673 .476 5.173 0.4 3.633	PH + O2 10.98 11.797 12.044 12.147 12.147 12.163 12.148 12.109	YOC6JDOA 8.023 8.909 9.203 9.347 9.401 9.418 9.42	PHOJ+O 1 12.728 13.332 13.39 13.402 73.407 13.41 13.413	ISOM (2<-1) C 13.556 13.793 13.491 13.243 13.122 13.069 13.041	6JYOO 13 4.888 3.637 1.824 -0.294 -2.168 -3.671 -5.211	SOM (1<-2) 15 13.531 13.753 13.426 13.15 13.01 12.947 12.913	GOM (3<- 2) Yi 12.31 12.737 12.632 12.528 12.478 12.458 12.449	OC6JDO -0.911 -4.481 -5.413 -6.098 -6.387 -6.713 -6.998	RODC6JDO 12.301 12.726 12.617 12.509 12.457 12.436 12.427	(OC5J+CO IS 7.958 8.66 8.869 8.995 9.06 9.095 9.122	OM (2<-3) 4.14 5.574 6.416 6.876 7.082 7.182 7.254	ISOM (4~3) 10.603 11.133 11.163 11.161 11.161 11.161 11.16 11.16	Y5JYO4DO -9.239 -8.725 -9.254 -9.543 -9.642 -9.678 -10.284	CY5J+CO2 10.6 11.128 11.153 11.146 11.142 11.14 11.138	ISOM (3<-4) 8.236 8.981 9.244 9.404 9.483 9.521 9.547	ISOM (5<-4) 8.397 9.134 9.388 9.543 9.619 9.656 9.681	YC50CJDO (-10,106 -9,554 -10,013 -10,001 -10,383 -10,008 -10,707	CY5J+CO2 IS 8.089 8.874 9.172 9.353 9.441 9.485 9.516	OM4 (4<-5) S 8,103 8,786 8,982 9,094 9,146 9,169 9,181	ium (forward) S 13,476 13,468 13,461 13,456 13,456 13,456 13,456 13,456	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
P (atm) 1.00E+00 1.00E+00 1.00E+00 1.00E+00 1.00E+00 1.00E+00 1.00E+00	T(K) 0 90 0 120 0 150 0 180 0 210 0 250	1000/T 20 1 20 1 20 0 20 0 20 0 20 0	PHOOJ .667 13.453 .111 13.05 .833 11.774 .667 9.91 .556 8.099 .476 6.611 0.4 5.093	PH + O2 5 10.386 2 11.705 5 12.039 1 12.147 9 12.163 9 12.146 2 12.109	YOC8JDOA 7.422 8.614 9.198 9.347 9.401 9.418 9.42	PHOJ+O 12.034 13.188 13.382 13.402 13.407 13.417 13.413	ISOM (2<-1) C 12.763 13.569 13.484 13.246 13.122 13.069 13.041	6JYOO 18 5.057 4.293 2.963 1.087 -0.738 -2.223 -3.75	50M (1<-2) 15 12.735 13.525 13.419 13.154 13.01 12.947 12.913	SOM (3<-2) 11.564 12.558 12.623 12.529 12.478 12.458 12.449	OC6JDO 5.841 3.48 0.503 -2.928 -5.291 -5.712 -5.998	RODC6JDO 11.555 12.546 12.608 12.51 12.457 12.436 12.427	YOC5J+CO 15 7.269 8.534 8.863 8.994 9.06 9.095 9.122	CM (2<-3) 3.626 5.528 6.414 6.876 7.081 7.182 7.254	ISOM (4~ 3) 9.883 10.981 11.154 11.161 11.161 11.16 11.16	Y5JY04D0 -8.961 -7.894 -8.262 -8.541 -8.642 -8.678 -9.283	CY5J+CO2 9.879 10.975 11.144 11.146 11.145 11.142 11.14 11.138	ISOM (3<-4) 7.561 8.865 9.238 9.404 9.483 9.521 9.547	ISOM (5<-4) 7.72 9.017 9.382 9.543 9.619 9.656 9.681	YC50CJD0 -4.565 -7.865 -9.02 -9.001 -9.383 -9.008 -9.707	CYSJ+CO2 IS 7.42 8.763 9.166 9.353 9.341 9.441 9.485 9.516	OM (4<-5) S 7.417 8.662 8.975 9.093 9.146 9.169 9.181	lum (forward) S 13.477 13.461 13.456 13.456 13.456 13.456 13.456 13.458	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
P (atm) 1.00E+0 1.00E+0 1.00E+0 1.00E+0 1.00E+0 1.00E+0 1.00E+0	T (K) 1 90 1 120 1 150 1 180 1 210 1 250	1000/T 00 1 00 1 00 0 00 0 00 0 00 0	PHOQJ .667 13.47 .111 13.34 .833 12.65 .667 11.15 .556 9.41 .476 7.95 0.4 6.44	PH + Q2 5 9.518 7 11.394 1 12.144 7 12.163 5 12.146 3 12.109	YOC6JDOA 6.551 8.497 9.157 9.344 9.401 9.418 9.42	PHOJ+O 11.123 12.794 13.322 13.399 13.407 13.41 13.413	ISOM (2<- 1) C 11.815 13.069 13.389 13.252 13.125 13.07 13.042	6JYOO (\$ 5.293 4.697 3.891 2.345 0.59 -0.881 -2.396	SOM (1<-2) 15 11.785 13.017 13.321 13.161 13.014 12.949 12.914	50M (3<- 2) Y 10.632 12.115 12.547 12.528 12.479 12.458 12.449	OC6JDO 9.045 8.241 6.586 3.906 1.119 -1.198 -3.608	RODC6JDO 10.612 12.102 12.532 12.51 12.458 12.436 12.427	YOC5J+CO IS 6.29 8.165 8.811 9.059 9.059 9.095 9.122	CM (2<-3) 2.716 5.312 6.394 6.872 7.08 7.181 7.253	ISOM (4<-3) 8.912 10.574 11.091 11.158 11.16 11.16 11.159	Y5JYO4DO -6.015 -7.302 -7.333 -7.536 -7.641 -7.678 -8.281	CY5J+CO2 8.906 10.567 11.081 11.144 11.142 11.14 13.138	ISOM (3<- 4) 6.582 8.513 9.191 9.4 9.482 9.52 9.546	ISOM (5<-4) 6.741 8.662 9.335 9.539 9.618 9.656 9.681	YC5OCJDO (0.521 -1.861 -4.169 -6.736 -8.336 -8.008 -8.706	CY5J+CO2 IS 6.441 8.417 9.121 9.349 9.44 9.484 9.515	CM (4<-5) 5 6.439 8.297 8.924 9.09 9.145 9.168 9.181	Sum (forward) S 13.477 13.474 13.462 13.456 13.456 13.456 13.456 13.456 13.458	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
P (atm) 2.00E+0/ 2.00E+0/ 2.00E+0/ 2.00E+0/ 2.00E+0/ 2.00E+0/ 2.00E+0/	T (K) 2 60 2 90 2 120 2 150 2 150 2 150 2 250	1000/F 00 1 00 1 00 0 00 0 00 0 00 0 00 0 00	PHOQJ .667 13.47 .111 13.46 .833 13.28 .867 12.5 .556 11.00 .476 9.57 .0.4 8.07	PH + Q2 7 8.242 5 10.51 5 11.697 1 12.101 2 12.156 4 12.143 7 12.108	YOC6.HDOA 5.274 7.608 8.851 9.3 9.395 9.415 9.418	PHOJ+O 9.837 11.831 12.949 13.352 13.405 13.41 13.413	ISOM (2<- 1) C 10.521 12.011 12.907 13.207 13.139 13.078 13.045	6.IYOO 18 6.105 5.037 4.584 3.707 2.156 0.708 -0.8	SOM (1<-2) 15 10.492 11.954 12.829 13.117 13.03 12.957 12.918	SOM (3<- 2) Y 9.333 11.105 12.123 12.48 12.483 12.461 12.451	OC6JDO 9.208 10.422 10.424 9.185 6.94 4.865 2.663	RODOBUDO 8.726 10.992 12.099 12.461 12.462 12.439 12.428	YOC5J+CO IS 4.295 7.044 8.423 8.924 9.044 9.086 9.117	OM (2<-3) 0.724 4.355 6.122 6.807 7.052 7.163 7.241	ISOM (4<-3) 6.951 9.439 10.673 11.096 11.153 11.155 11.157	Y5JYO4DO 0.122 -0.852 -1.951 -3.692 -5.995 -6.364 -6.941	CY5J+CO2 6.948 9.431 10.681 11.081 11.135 11.137 11.136	ISOM (3<- 4) 4.575 7.402 8.817 9.333 9.464 9.51 9.54	ISOM (5<- 4) 4.734 7.55 8.959 9.472 9.601 9.646 9.674	YCSOCJDO 3.208 2.93 1.183 -0.441 -2.53 -4.435 -6.42	CY5J+CO2 IS 4.394 7.308 8.751 9.281 9.421 9.474 9.509	OM (4<-5) 5 4.445 7.179 8.539 9.023 9.13 9.16 9.176	6um (forward) 5 13.477 13.477 13.458 13.456 13.456 13.457 13.458	Sum (ail) 13.477 13.477 13.477 13.477 13.477 13.477 13.477 13.477
T (K) 60 60 60 60 60 60	kog P (antr 0 0 0 0 0 0 0 0 2.30	m) PHOQJ -3 12 -2 13 -1 13 0 13 1 13 01 13	PH + O2 .398 11.322 .039 11.22 .352 10.94 .455 10.388 .475 9.511 .477 8.24	YOC6JDOA 5 8.38 5 8.302 9 8.023 5 7.422 3 6.551 2 5.274	PHOJ+0 13.259 13.115 12.728 12.034 11.123 9.837	SOM (2<-1) 14.324 14.079 13.556 12.763 11.815 10.521	C6JYOO IS 3.923 4.565 4.888 5.057 5.293 6.105	OM (1<-2) 1 14.305 14.057 13.531 12.735 11.785 10.492	SOM (3<- 2) Y 12.961 12.767 12.31 11.564 10.632 9.333	OC6JDO R -6.501 -5.753 -0.911 5.841 9.045 9.208	ODC6JDO 12.954 12.759 12.301 11.555 10.612 8.726	YOC5J+CO 8.492 8.344 7.959 7.269 6.29 4.295	SOM (2<- 3) IS 4.401 4.349 4.14 3.626 2.716 0.724	COM (4<-3) 11.197 11.026 10.803 9.883 8.912 6.951	Y5.W04D0 -10,624 -9.819 -9.239 -8.961 -6.015 0,122	CY5J+CO2 11,194 11,023 10,6 9,879 8,908 6,948	ISOM (3~ 4) 8.743 8.605 8.236 7.561 6.582 4.575	ISOM (5<- 4) 8.907 8.768 8.397 7.72 6.741 4.734	YC50CJD0 -11.5 -10.692 -10.106 -4.565 0.521 3.208	CY5J+CO2 8.582 8.449 8.069 7.42 6.441 4.394	SOM (4<-5) S 8.629 8.484 8.103 7.417 6.439 4.445	um (forward) 5 13.474 13.475 13.476 13.476 13.477 13.477 13.477	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477	
T (K) 90 90 90 90 90 90	kog P (atr 0 0 0 0 0 0 2.34	m) PHOOJ -3 10 -2 11 -1 12 0 1 1 13 01 13	PH + O2 187 11.81 438 11.81 386 11.79 3.02 11.70 347 11.39 465 10.5	YOO&JDOA 5 8.927 7 8.909 5 8.814 4 8.497 1 7.608	PHO/+O 13.366 13.363 13.332 13.188 12.794 11.831	SOM (2<- 1) 13.851 13.849 13.793 13.569 13.069 12.011	C&JYOO IS 1.435 2.688 3.637 4.293 4.697 5.037	60M (1<-2) 1 13.812 13.811 13.753 13.525 13.017 11.954	SOM (3<- 2) Y 12.784 12.779 12.737 12.558 12.115 11.105	OC6JDO R -7.02 -6.021 -4.481 3.48 8.241 10.422	ODC6JDO 12.773 12.769 12.726 12.546 12.102 10.992	YOC5J+CO 8.689 8.686 8.534 8.165 7.044	ISOM (2<-3) (5 5.581 5.58 5.574 5.528 5.312 4.355	OM (4<- 3) 11.171 11.167 11.133 10.981 10.574 9.439	Y5JYO4DO -10.684 -9.687 -8.725 -7.894 -7.302 -0.852	CY5J+CO2 11.166 11.162 11.128 10.975 10.567 9.431	ISOM (3<-4) 9.007 9.004 8.981 8.865 8.513 7.402	ISOM (5<- 4) 9.16 9.157 9.134 9.017 8.662 7.55	YCSOCJDO -11.522 -10.526 -9.554 -7.865 -1.861 2.93	CY5J+CO2 8.899 8.896 8.874 8.763 8.417 7.308	SOM (4<- 5) S 8.815 8.812 8.786 8.662 8.297 7.179	um (forward) 5 13.468 13.468 13.468 13.47 13.474 13.477	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477	
T (K) 120 120 120 120 120 120	tog,P(atr 0 0 0 0 0 0 2.3	m) PHOOJ -3 1 -2 6 -1 10 0 11 1 12 01 13	PH + O2 7.698 12.04 9.266 12.04 9.628 12.04 9.628 12.04 1.778 12.03 9.651 1 9.285 11.69	YOC&JDOA 5 9.204 5 9.204 4 9.203 9 9.198 2 9.157 7 8.851	PHOJ+O 13.391 13.391 13.39 13.382 13.322 13.322 12.949	ISOM (2<-1) 13.486 13.487 13.491 13.484 13.389 12.907	C6JYOO IS +1.107 0.46 1.824 2.983 3.891 4.584	50M (1<-2) 15 13.42 13.422 13.426 13.419 13.321 12.829	SOM (3<- 2) 1 12.632 12.632 12.632 12.632 12.623 12.547 12.123	OC8UDO R -7.415 -6.415 -5.413 0.503 6.586 10.424	CODC6JDO 12.617 12.617 12.617 12.608 12.532 12.099	YOC5J+CO 8.87 8.869 8.863 8.811 8.423	ISOM (2<-3) IS 6.417 6.417 6.416 6.414 6.394 6.122	OM (4<-3) 11.163 11.163 11.163 11.163 11.154 11.091 10.673	Y5JYO4DO -11,254 -10,254 -9,254 -8,262 -7,333 -1,951	CY5J+CO2 11.153 11.153 11.153 11.153 11.144 11.081 10.661	ISOM (3~ 4) 9.245 9.244 9.244 9.238 9.191 8.817	ISOM (5<- 4) 9.389 9.369 9.388 9.388 9.382 9.335 8.959	YC50CJD0 -12.012 -11.012 -10.013 -9.02 -4.169 1.183	CY5J+CO2 9.173 9.173 9.172 9.166 9.121 8.751	SOM (4 <- 5) S 8.982 8.982 8.982 8.975 8.924 8.539	um (forward) 5 13.461 13.461 13.461 13.461 13.462 13.47	Sum (all) 13.477 13.477 13.477 13.477 13.477 13.477 13.477	

Mar 2001 (chemast) PH + O2 => Products low for sensitivity ChemMaster chemact output for mac spreadsheet

Low jwb / N sebar

APPENDIX

reactants: PH + O2

T (K)	ka	q P (alm)	PHOOJ	PH+	02 Y	/OC6JDOA	PHOJ+0	ISOM (2<- 1)	CEJYOO	ISOM (1<-2)	SOM (3<- 2)	YOC6JDO	RODC6JDO	YOC5J+CO	ISOM ('2<-3)	ISOM (4<-3)	Y5JY04DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	AC20CYD0	CY5J+CO2	ISOM (4~ 5)	Sum (forward) Su	um (ali)
· · · ,	1500	°-3	5	354	12.147	9.347	13.402	13.24	2 -3.476	13.149	12.528	-8.101	12,509	6.995	6.876	11.161	-11.543	11.146	i 9.404	9.543	-12.001	9.353	9.094	13.456	13.477
	1500	-2	7	028	12.147	9.347	13.402	13.24	3 -1.802	13.149	12,528	-7.1	12,509	8.995	5 6.876	11.161	-10.543	11.146	9.404	9.543	-11.00°	9.353	9.094	13.456	13.477
	500	-1	8	535	12.147	9.347	13.402	13.24	3 -0.294	13,15	12.528	-6.096	12,509	8.99	6.876	11.161	-9.543	11.14E	9.404	9.543	-10.00°	9.353	9.094	13.456	13.477
	1500	0	9	911	12.147	9.347	13.402	13.246	5 1.067	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	13.25	2 2.345	13.161	12.528	3.906	12.51	8.99	6.872	11.158	-7.536	11.144	9.4	9.539	-6.736	9.349	9.09	13.456	13.477
	1500	2.301	1	2.51	12.101	9.3	13.352	13.20	3.707	13.117	12.48	9.185	12.461	8.924	6.807	11.096	-3.692	11.081	9.333	9.472	-0.44	9.281	9.023	13.458	13.477
T (K)	ko	o P (aim)	PHOOJ	PH+	02 Y	ADDLaDON	PHOJ+0	ISOM (2 - 1	CEJYOO	ISOM (1<-2)	SOM (3<- 2)	YOOGJDO	RODC6JDO	YOCSHCO	ISOM (2<- 3)	SOM { 4<- 3}	Y5JYO4DO	CY5J+CO2	ISOM (3~4)	ISOM (5<- 4)	YCSOCJDO	CY5J+CO2	ISOM (4<- 5)	Sum (forward) Su	um (all)
	1800	-3	:	3.41	12.163	9.401	13.407	13.12	-5.43	13.009	12.478	-8.388	12.457	9.06	3 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	13.12	2 -3.717	13,01	12.478	-7.388	12.457	9.0	5 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	13.12	2 -2.168	13.01	12,478	-6.387	12.457	9.0	5 7.082	11.161	-9.642	11.142	9.483	9.619	-10.383	3 9.441	9.146	13.456	13.477
	1800	D	8	099	12.163	9.401	13.407	13.12	2 -0.736	13.01	12.478	-5.291	12.457	9.0	5 7.081	11,161	-8.642	11.142	9.483	9.619	-9.36	3 9.441	9.146	13.456	13.477
	1800	1	9	417	12.163	9.401	13.407	13.12	5 0.59	13.014	12.479	1,119	12.458	9.05	9 7.06	11.1E	-7,641	11.142	9.482	9.610	3 -8.33	3 9.44	9.145	13.456	13.477
	1800	2.301	11	002	12.156	9.395	13.405	5 13.13	2.156	13.03	12.483	6.94	12.462	9.044	1 7.052	11.153	-5.995	i 11.135	9.464	9.601	-2.53	9.421	9.13	13.456	13.477
TAN		n D (alm)	PHOOI	DH +	02 1		PHO HO	ISOM (2<-1	06800	ISOM (15-2)	SOM (3c. 2)	Y006/00	RODCELDO	Y005.000	ISOM (2<- 3)	ISOM (4<- 3)	Y5.NO4DO	CY5J+CO2	ISOM (3<- 4)	ISOM (5<- 4)	YC50CJD0	CY5J+CO2	ISOM (4<-5)	Sum (forward) Se	um (all)
1 (15)	2100	-gr= (asin) - 3	1	867	12 146	9418	13.41	13.06	A	12 947	12 458	-8 713	12 4 36	9.09	5 7 182	11 16	-11.678	11.14	9.521	9.65	-12.00	3 9,485	9,169	13,458	13.477
	2100	.2	3	605	12 146	9.418	13.41	13.06	-5.239	12.947	12,458	-7 713	12.436	9.09	5 7.182	11.16	-10.678	3 11.14	9.521	9.65	5 -11.004	9,485	i 9.169	13.456	13.477
	2100		5	173	12 146	9 4 18	13.41	13.06	-3671	12.947	12 458	-6 713	12 4 36	9 095	5 7.182	11.16	-9.676	11.14	9.521	9.656	3 -10.006	9.485	9.169	13.456	13.477
	2100	0	ě	619	12.146	9.418	13.41	13.06	-2.223	12.947	12 458	-5.712	12.436	9.09	5 7.182	11.16	-8.678	11.14	9.521	9.656	3 -9.008	3 9,485	9.169	13.456	13.477
	2100	1	7	955	12 146	9.418	13.41	13.0	7 -0.881	12,949	12.458	-1.198	12 4 36	9.09	5 7.181	11.16	-7.678	3 11.14	9.52	9.65	5 -8.004	3 9.484	9.166	13.456	13.477
Ē	2100	2.301	9	574	12.143	9.415	13.41	13.07	8 0.706	12.957	12.461	4.865	12.439	9.06	6 7.163	11.156	5 -6.364	11.13	9.51	9.64	5 -4.43	5 9.474	9.16	13.457	13.477
1 10		n P (atm)	PHOOL	PH +	02 1		PHO.HO	ISOM (2<- 1	CANOO	ISOM (15-2)	ISOM (3<- 2)	YOC6.000	800C6.ID0	YOCSHCO	ISOM (25-3)	ISOM (4<- 3)	Y5.NO4DO	CY5.HC02	ISOM (3<- 4)	ISOM (5<- 4)	YCSOCJDO	CY5J+CO2	ISOM (4 - 5)	Sum (forward) Se	um (all)
1 (14)	2600	-3 -3	11000	284	12 109	942	13 413	13.04	1 -8 54	12 913	12 449	-8 998	12 4 27	9.12	3 7 254	11.16	-12.284	11.138	9.547	9.68	-12.70	7 9.516	9.181	13.458	13.477
	2500		ž	047	12 109	942	13 413	13.04	6794	12 913	12 449	-7 998	12 427	9 12	3 7 254	11.16	-11.284	11.138	9.547	9.68	-11.70	7 9.516	9,181	13,458	13.477
	1600			£10	12 100	9.42	13 4 13	13.04	1 .5211	12 013	12 449	-6 998	12 4 27	9.12	7 7 254	11.16	-10 284	11.13	9 547	9.68	-10.70	7 9.516	9 181	13,458	13,477
	2500		š	002	12 109	942	13 4 1 3	13.04	1 .374	12.913	12 449	-5 998	12 427	9.12	2 7 254	11.16	-9.28	11.13	9.547	9.68	1 -9.70	7 9.516	9.181	13,458	13.477
	2500	1	5	443	12 109	942	13 4 13	13.04	2 394	12 914	12 449	-3 608	17 427	9 12	2 7 253	11 159	-8.281	11.138	9,546	9.68	-8.70	3 9,515	9.181	13.458	13.477
ł	2500	2.301	8	077	12.108	9.418	13.413	13.04	5 -0.8	12.918	12.451	2.663	12.428	9.11	7 7.241	11.15	-6.941	1 11.136	9.54	9.67	-6.4	9.509	9.176	13.458	13.477

ChemMaster dissoc output for mac spreadsheet

reactants: PHOOJ

P (atm)	Т (К)	1000/T	PH +	02	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-03	600	1.0	667	-6.153	-9.105	-4.495	-3.979	-3.861
1.00E-03	900	1.1	111	-0.436	-3.295	1.363	1.897	2.01
1.00E-03	1200	0.8	333	1.503	-1.289	3.402	3.95	4.059
1.00E-03	1500	0.0	667	2.152	-0.588	4.128	4.687	4.794
1.00E-03	1800	0.9	556	2.373	-0.325	4.413	4.98	5.085
1.00E-03	2100	0.4	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)	т (К)	1000/T	PH +	02	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-02	600	1.0	667	-5.203	-8.155	-3.549	-3.037	-2.918
1.00E-02	900	1.1	111	0.543	-2.315	2.339	2.871	2.984
1.00E-02	1200	0.8	333	2.491	-0.3	4.388	4.934	5.044
1.00E-02	1500	0.6	67	3.144	0.404	5.119	5.676	5.784
1.00E-02	1800	0.9	556	3.368	0.67	5.407	5.973	6.078
1.00E-02	2100	0.4	176	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)	Т (К)	1000/T	PH +	02	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E-01	600	1.6	67	-4.453	-7.406	-2.82	-2.326	-2.202
1.00E-01	900	1.1	111	1.417	-1.442	3.193	3.708	3.825
1.00E-01	1200	0.8	333	3.415	0.623	5.295	5.827	5.94
1.00E-01	1500	0.6	67	4.093	1.352	6.053	6.598	6.708
1.00E-01	1800	0.5	556	4.33	1.632	6.357	6.913	7.02
1.00E-01	2100	0.4	76	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)	Т (К)	1000/T	PH +	02	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E+00	600	1.6	67	-4.04	-6.999	-2.447	-1.98	-1.849
1.00E+00	900	1.1	11	2.091	-0.777	3.799	4.267	4.397
1.00E+00	1200	3.0	333	4.209	1.407	6.015	6.495	6.621
1.00E+00	1500	0.6	67	4.943	2.193	6.831	7.326	7.448
1.00E+00	1800	0.5	556	5.211	2.504	7.169	7.677	7.796
1.00E+00	2100	0.4	76	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)	Т (К)	1000/T	PH +	02	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
1.00E+01	600	1.6	67	-3.913	-6.874	-2.341	-1.888	-1.754
1.00E+01	900	1.1	11	2.539	-0.339	4.158	4.565	4.712
1.00E+01	1200	3.0	333	4.915	2.099	6.585	6.965	7.119
1.00E+01	1500	0.6	67	5.775	3.01	7.506	7.881	8.036
1.00E+01	1800	0.5	556	6.106	3.382	7.896	8.274	8.428
1.00E+01	2100	0.4	76	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)	Т (К)	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
	Т (К)	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
	Т (К)	log P (atm)	PH + O2	YOC6JDOA	PHOJ+O	C6JYOO	QRRK (tot)
	<u> </u>	-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
	Т (К)	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
	Т (К)	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
	Т (К)	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

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

ChemMaster dissoc output for mac spreadsheet

reactants: C6JYOO

P (atm)	т (К)	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)	Т (К)	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)	Т (К)	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)	т (К)	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)	Т (К)	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)	Т (К)	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
	Т (К)	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
	Т (К)	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
	Т (К)	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

Т (К)	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
т (К)	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
т (К)	log P (atm)	PHOQU	YOCAIDO	ORRK (tot)
T (K) 2100	log P (atm)	PHOOJ 5 134	YOC6JDO	QRRK (tot) 5 224
T (K) 2100 2100	log P (atm) -3 -2	PHOOJ 5.134 6 134	YOC6JDO 4.496 5.496	QRRK (tot) 5.224 6 224
T (K) 2100 2100 2100	log P (atm) -3 -2 -1	PHOOJ 5.134 6.134 7 134	YOC6JDO 4.496 5.496 6.496	QRRK (tot) 5.224 6.224 7 224
T (K) 2100 2100 2100 2100	log P (atm) -3 -2 -1	PHOOJ 5.134 6.134 7.134 8.134	YOC6JDO 4.496 5.496 6.496 7.496	QRRK (tot) 5.224 6.224 7.224 8 224
T (K) 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1	PHOOJ 5.134 6.134 7.134 8.134 9.134	YOC6JDO 4.496 5.496 6.496 7.496 8.496	QRRK (tot) 5.224 6.224 7.224 8.224 9.224
T (K) 2100 2100 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512
T (K) 2100 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512
T (K) 2100 2100 2100 2100 2100 2100 T (K)	log P (atm) -3 -2 -1 0 1 2.301 log P (atm)	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot)
T (K) 2100 2100 2100 2100 2100 2100 T (K) 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ 5.22	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO 4.58	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot) 5.31
T (K) 2100 2100 2100 2100 2100 2100 T (K) 2500 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ 5.22 6.22	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO 4.58 5.58	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot) 5.31 6.31
T (K) 2100 2100 2100 2100 2100 2100 2100 T (K) 2500 2500 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ 5.22 6.22 7.22	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO 4.58 5.58 6.58	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot) 5.31 6.31 7.31
T (K) 2100 2100 2100 2100 2100 2100 2100 2500 25	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ 5.22 6.22 7.22 8.22	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO 4.58 5.58 6.58 7.58	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot) 5.31 6.31 7.31 8.31
T (K) 2100 2100 2100 2100 2100 2100 2100 T (K) 2500 2500 2500 2500 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1	PHOOJ 5.134 6.134 7.134 8.134 9.134 10.422 PHOOJ 5.22 6.22 7.22 8.22 9.22	YOC6JDO 4.496 5.496 6.496 7.496 8.496 9.784 YOC6JDO 4.58 5.58 6.58 7.58 8.579	QRRK (tot) 5.224 6.224 7.224 8.224 9.224 10.512 QRRK (tot) 5.31 6.31 7.31 8.31 9.309

ChemMaster dissoc output for mac spreadsheet

reactants: YOC6JDO

P (atm)	Т (К)	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)	Т (К)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E-02	600	1.66	7 3.1	-10.846	-34.987	-2.952	3.1
1.00E-02	900	1.11	1 5.265	-8.022	-29.973	-0.368	5.265
1.00E-02	1200	0.83	3 5.924	-7.282	-28.077	0.347	5.924
1.00E-02	1500	0.66	6.126	-7.123	-27.186	0.525	6.126
1.00E-02	1800	0.55	5.798	-7.707	-27.296	0.035	5.798
1.00E-02	2100	0.47	5 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)	Т (К)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E-01	600	1.66	7 3.261	-8.159	-26.081	-2.036	3.261
1.00E-01	900	1.11	1 5.857	-4.47	-21.523	1.247	5.857
1.00E-01	1200	0.83	3 6.637	-3.497	-20.29	2.155	6.637
1.00E-01	1500	0.66	7 6.884	-3.269	-19.983	2.406	6.884
1.00E-01	1800	0.55	5 7.001	-3.203	-19.865	2.507	7.001
1.00E-01	2100	0.47	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)	Т (К)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E+00	600	1.66	7 3.309	-7.022	-19.331	-1.669	3.309
1.00E+00	900	1.11	6.261	-2.3	-13.482	2.355	6.261
1.00E+00	1200	0.83	3 7.262	-0.884	-11.935	3.607	7.262
1.00E+00	1500	0.66	7 7.614	-0.425	-11.575	4.024	7.614
1.00E+00	1800	0.55	5 7.767	-0.263	-11,579	4.185	7.767
1.00E+00	2100	0.47	5 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)	Т (К)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
1.00E+01	600	1.66	7 3.317	-6.698	-16.662	-1.582	3.317
1.00E+01	900	1.11	l 6.47	-1.074	-8.866	2.977	6.47
1.00E+01	1200	0.83	3 7.763	0.976	-6.273	4.709	7.763
1.00E+01	1500	0.66	7 8.268	1.736	-5.385	5.357	8.269
1.00E+01	1800	0.55	6 8.494	2.053	-5.08	5.63	8.495
1.00E+01	2100	0.47	6 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)	Т (К)	1000/T	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
2.00E+02	600	1.66	7 3.318	-6.644	-16.014	-1.57	3.318
2.00E+02	900	1.11	6.534	-0.575	-6.696	3.205	6.535
2.00E+02	1200	0.83	8.112	2.278	-2.546	5.488	8.113
2.00E+02	1500	0.66	7 8.921	3.651	-0.656	6.61	8.924
2.00E+02	1800	0.55	§ 9.325	4.308	0.218	7.15	9.328
2.00E+02	2100	0.47	§ 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

Т (К)	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
т (К)	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
Т (К)	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
Т (К)	log P (atm)	RODC6JDO	YOC5J+CO	C6JYOO	Y5JYO4DO	QRRK (tot)
T (K) 1500	log P (atm) -3	RODC6JDO 5.331	YOC5J+CO -11.4	C6JYOO -32.228	Y5JYO4DO -1.954	QRRK (tot) 5.331
T (K) 1500 1500	log P (atm) -3 -2	RODC6JDO 5.331 6.126	YOC5J+CO -11.4 -7.123	C6JYOO -32.228 -27.186	Y5JYO4DO -1.954 0.525	QRRK (tot) 5.331 6.126
T (K) 1500 1500 1500	log P (atm) -3 -2 -1	RODC6JDO 5.331 6.126 6.884	YOC5J+CO -11.4 -7.123 -3.269	C6JYOO -32.228 -27.186 -19.983	Y5JYO4DO -1.954 0.525 2.406	QRRK (tot) 5.331 6.126 6.884
T (K) 1500 1500 1500 1500	log P (atm) -3 -2 -1 0	RODC6JDO 5.331 6.126 6.884 7.614	YOC5J+CO -11.4 -7.123 -3.269 -0.425	C6JYOO -32.228 -27.186 -19.983 -11.575	Y5JYO4DO -1.954 0.525 2.406 4.024	QRRK (tot) 5.331 6.126 6.884 7.614
T (K) 1500 1500 1500 1500 1500	log P (atm) -3 -2 -1 0 1	RODC6JDO 5.331 6.126 6.884 7.614 8.268	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357	QRRK (tot) 5.331 6.126 6.884 7.614 8.269
T (K) 1500 1500 1500 1500 1500 1500	log P (atm) -3 -2 -1 0 1 2.301	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924
T (K) 1500 1500 1500 1500 1500 1500 T (K)	log P (atm) -3 -2 -1 0 1 2.301 log P (atm)	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot)
T (K) 1500 1500 1500 1500 1500 T (K) 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06
T (K) 1500 1500 1500 1500 1500 T (K) 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798
T (K) 1500 1500 1500 1500 1500 T (K) 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1800 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1800 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328
T (K) 1500 1500 1500 1500 1500 T (K) 1800 1800 1800 1800 1800 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm)	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot)
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1500 1800 180	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO 5.103	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO -11.612	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO -31.296	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO -2.421	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot) 5.103
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1900	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO 5.103 5.846	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO -11.612 -7.758	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO -31.296 -26.977	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO -2.421 0.019	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot) 5.103 5.846
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1900	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO 5.103 5.846 6.632	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO -11.612 -7.758 -3.859	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO -31.296 -26.977 -20.612	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO -2.421 0.019 1.986	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot) 5.103 5.846 6.632
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 1900 1500 1800 2100 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO 5.103 5.846 6.632 7.86	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO -11.612 -7.758 -3.859 -0.194	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO -31.296 -26.977 -20.612 -11.688	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO -2.421 0.019 1.986 4.267	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot) 5.103 5.846 6.632 7.86
T (K) 1500 1500 1500 1500 1500 1500 T (K) 1800 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	RODC6JDO 5.331 6.126 6.884 7.614 8.268 8.921 RODC6JDO 5.06 5.798 7.001 7.767 8.494 9.325 RODC6JDO 5.103 5.846 6.632 7.86 8.617	YOC5J+CO -11.4 -7.123 -3.269 -0.425 1.736 3.651 YOC5J+CO -11.688 -7.707 -3.203 -0.263 2.053 4.308 YOC5J+CO -11.612 -7.758 -3.859 -0.194 2.205	C6JYOO -32.228 -27.186 -19.983 -11.575 -5.385 -0.656 C6JYOO -31.851 -27.296 -19.865 -11.579 -5.08 0.218 C6JYOO -31.296 -26.977 -20.612 -11.688 -4.997	Y5JYO4DO -1.954 0.525 2.406 4.024 5.357 6.61 Y5JYO4DO -2.381 0.035 2.507 4.185 5.63 7.15 Y5JYO4DO -2.421 0.019 1.986 4.267 5.766	QRRK (tot) 5.331 6.126 6.884 7.614 8.269 8.924 QRRK (tot) 5.06 5.798 7.001 7.767 8.495 9.328 QRRK (tot) 5.103 5.846 6.632 7.86 8.618

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Т (К)	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

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reactants: Y5JYO4DO

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P (atm)	т (К)	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)	Т (К)	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)	Т (К)	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)	Т (К)	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

P (atm)	т (К)	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	0.550	9.904	-2.000	2.230	0.004
	2100	0.470	9.909	-2.039	-2.213	9.909
1.00E+01	2000	0.4	9.904	-2.011	-2.109	9.904
	T (10)	4000 		VOCEIDO		
	1 (K) 000	1000/1	0.700	TUCOJDU	10000000	
2.00E+02	600	1.007	9.726	0.582	0.957	9.720
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
	Т (К)	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
	000	2.501	5.720	0.002	0.007	0.720
	T (K)	log P (atm)	CY5 I+CO2			ORRK (tot)
		-3 IOG 1	5.87	-10 579	-10 144	5.87
	900	-5	5.07	-10.579	-10.144	5.07 6.960
	900	-2	0.009	-9.572	-9.137	0.009
	900	-1	7.800	-8.501	-0.000	7.000
	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
	т (К)	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
	Т (К)	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

Т (К)	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
Т (К)	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
Т (К)	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)	т (К)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
1.00E-03	600	1.66	7 2.133	2.821	2.902
1.00E-03	900	1.11	1 4.172	4.831	4.918
1.00E-03	1200	0.83	3 4.679	5.317	5.407
1.00E-03	1500	0.66	7 4.853	5.475	5.568
1.00E-03	1800	0.55	6 4.929	5.539	5.634
1.00E-03	2100	0.47	6 4.966	5.565	5.662
1.00E-03	2500	0.	4 4.988	5.575	5.675
P (atm)	Т (К)	1000/T	CY5J+CO2	Y5JYO4DO	QRRK (tot)
P (atm) 1.00E-02	T (K) 600	1000/T 1.66	CY5J+CO2 7 3.132	Y5JYO4DO 3.82	QRRK (tot) 3.901
P (atm) 1.00E-02 1.00E-02	T (K) 600 900	1000/T 1.66 1.11	CY5J+CO2 7 3.132 1 5.172	Y5JYO4DO 3.82 5.831	QRRK (tot) 3.901 5.917
P (atm) 1.00E-02 1.00E-02 1.00E-02	T (K) 600 900 1200	1000/T 1.66 1.11 0.83	CY5J+CO2 7 3.132 1 5.172 3 5.679	Y5JYO4DO 3.82 5.831 6.317	QRRK (tot) 3.901 5.917 6.407
P (atm) 1.00E-02 1.00E-02 1.00E-02 1.00E-02	T (K) 600 900 1200 1500	1000/T 1.66 1.11 0.83 0.66	CY5J+CO2 7 3.132 1 5.172 3 5.679 7 5.853	Y5JYO4DO 3.82 5.831 6.317 6.475	QRRK (tot) 3.901 5.917 6.407 6.568
P (atm) 1.00E-02 1.00E-02 1.00E-02 1.00E-02 1.00E-02	T (K) 600 900 1200 1500 1800	1000/T 1.66 1.11 0.83 0.66 0.55	CY5J+CO2 7 3.132 1 5.172 3 5.679 7 5.853 6 5.928	Y5JYO4DO 3.82 5.831 6.317 6.475 6.538	QRRK (tot) 3.901 5.917 6.407 6.568 6.634
P (atm) 1.00E-02 1.00E-02 1.00E-02 1.00E-02 1.00E-02 1.00E-02	T (K) 600 900 1200 1500 1800 2100	1000/T 1.66 1.11 0.83 0.66 0.55 0.47	CY5J+CO2 7 3.132 1 5.172 3 5.679 7 5.853 6 5.928 6 5.966	Y5JYO4DO 3.82 5.831 6.317 6.475 6.538 6.565	QRRK (tot) 3.901 5.917 6.407 6.568 6.634 6.662

P (atm)	Т (К)	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)	Т (К)	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)	Т (К)	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)	Т (К)	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
	т (К)	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

Т (К)	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 (stm)			ORRK (tot)
1200	-3 -3	4 679	5 317	5 407
1200	-2	5 679	6 317	6.407
1200		6 676	7 314	7 404
1200	-1	7 651	8 283	8 374
1200	1	P.517	0.203	0.014
1200	2 201	0.017	9.114	9.212
1200	2.301	9.412	9.074	10.005
Т (К)	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 (10)	la a D (atas)			
т (К)	log P (atm)	CY5J+CO2	Y5JYO4DO	QRRK (tot)
T (K) 1800	log P (atm) -3	CY5J+CO2 4.929	Y5JYO4DO 5.539	QRRK (tot) 5.634
T (K) 1800 1800	log P (atm) -3 -2	CY5J+CO2 4.929 5.928	Y5JYO4DO 5.539 6.538	QRRK (tot) 5.634 6.634
T (K) 1800 1800 1800	log P (atm) -3 -2 -1	CY5J+CO2 4.929 5.928 6.927	Y5JYO4DO 5.539 6.538 7.536	QRRK (tot) 5.634 6.634 7.632
T (K) 1800 1800 1800 1800	log P (atm) -3 -2 -1 0	CY5J+CO2 4.929 5.928 6.927 7.913	Y5JYO4DO 5.539 6.538 7.536 8.518	QRRK (tot) 5.634 6.634 7.632 8.614
T (K) 1800 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1	CY5J+CO2 4.929 5.928 6.927 7.913 9.845	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335	QRRK (tot) 5.634 6.634 7.632 8.614 10.457
T (K) 1800 1800 1800 1800 1800 1800	log P (atm) -3 -2 -1 0 1 2.301	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717
T (K) 1800 1800 1800 1800 1800 1800 1800 T (K)	log P (atm) -3 -2 -1 0 1 2.301 log P (atm)	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot)
T (K) 1800 1800 1800 1800 1800 1800 T (K) 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662
T (K) 1800 1800 1800 1800 1800 1800 T (K) 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662
T (K) 1800 1800 1800 1800 1800 1800 T (K) 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661
T (K) 1800 1800 1800 1800 1800 1800 1800 T (K) 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646
T (K) 1800 2100 200 2	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 2100 2100 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763
T (K) 1800 1800 1800 1800 1800 1800 1800 T (K) 2100 2100 2100 2100 2100 2100 2100	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 1800 2100 200 2	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm)	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot)
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 1800 2100 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -3	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2 4.988	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO 5.575	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot) 5.675
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 2100 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2 4.988 5.988	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO 5.575 6.575	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot) 5.675 6.675
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 2100 2500 200 2	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -3 -2 -1	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2 4.988 5.988 6.987	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO 5.575 6.575 7.574	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot) 5.675 6.675 7.674
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 2100 2100 2100 2100 2100 2100 2100 2100 2100 2500 2500 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2 4.988 5.988 6.987 7.978	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO 5.575 6.575 7.574 8.561	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot) 5.675 6.675 7.674 8.662
T (K) 1800 1800 1800 1800 1800 1800 1800 1800 2100 2100 2100 2100 2100 2100 2100 2100 2100 2500 2500 2500 2500	log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301 log P (atm) -3 -2 -1 0 1 2.301	CY5J+CO2 4.929 5.928 6.927 7.913 9.845 10.241 CY5J+CO2 4.966 5.966 6.964 7.953 9.881 10.297 CY5J+CO2 4.988 5.988 6.987 7.978 9.908	Y5JYO4DO 5.539 6.538 7.536 8.518 10.335 10.541 Y5JYO4DO 5.565 6.565 7.563 8.548 10.365 10.581 Y5JYO4DO 5.575 6.575 7.574 8.561 10.386	QRRK (tot) 5.634 6.634 7.632 8.614 10.457 10.717 QRRK (tot) 5.662 6.662 7.661 8.646 10.488 10.763 QRRK (tot) 5.675 6.675 7.674 8.662 10.511

Modified Arrhenius fits of the rate constants for the product channels of phenyl + 02 and its stable products

Mar 2001	(chemast) PH + 02 -> Products	low for	gengitiv	itv		Low	iwh / N	sehar				
PH + 02		1.03+107	-30.86	24144	1	1 00E-03 a	tm. 60	0-2500 K	44%	err	··CM	
PH + 02	C=> PHOOT	6 34+114	-32 44	31730	i	1 00E-02 a	tm. 60	0-2500 к,	45%	err	• • CM	
PH + 02	<=> PHOOJ	4 75+122	-34 07	40095	;	1.00E-01 a	tm 60.	0-2500 K,	41%	err	· · CM	:
	C-> PHOOJ	8 76+127	-34 99	47402	ì	1 00E+00 a	tm 60	0-2500 K,	328	err	• • CM	:
	C-> PHOOD	2 22,127	-34.33	E1202.	,	1.00E+00 a	tm = 60	0-2500 K,	128	arr	· · · · · · ·	2
PH + O2		1 21,116	-34.33	19965	:	2 00E+01 a	tm 60	0-2500 K,	029	orr	CM	:
PH + 02		1.017.10	-30.47	49000.	1	2.00E+02 a	tm 60	0-2500 K,	ດລາ ຈາຍ	err	: CM	
PH + 02	<=> PH + 02	1.086+19	-1.05	7075.	÷	1.00E-03 a	till, 60	0-2500 K,	37 08	err	::CM	•
PH + 02	<=> PH + U2	1.198+20	-2.14	/94/.		1.00E-02 a	Cm, 60	0-2500 K,	21	err	::CM	:
PH + OZ	<=> PH + O2	5.86E+23	-3.15	11064.	!	1.00E-01 a	tm, 60	0-2500 K,	28	err	::CM	:
PH + O2	<=> PH + O2	1.186+31	-5.15	17472.	1	1.00E+00 a	cm, 60	0-2500 K,	98	err	::CM	:
PH + 02	<=> PH + O2	1.17E+39	-7.30	25376.	1	1.00E+01 a	tm, 60	0-2500 K,	11%	err	::CM	:
PH + O2	<=> PH + O2	3.44E+41	-7.84	31725.	!	2.00E+02 a	tm, 60	0-2500 K,	16%	err	::CM	:
PH + 02	<=> YOC6JDOA	1.94E+14	-1.26	6662.	!	1.00E-03 a	tm, 60	0-2500 K,	38	err	::CM	:
PH + 02	<=> YOC6JDOA	2.42E+15	-1.56	7577.	!	1.00E-02 a	tm, 60	0-2500 K,	28	err	::CM	:
PH + 02	<=> YOC6JDOA	1.49E+19	-2.60	10779.	1	1.00E-01 a	tm, 60	0-2500 K,	38	err	::CM	:
PH + O2	<=> YOC6JDOA	3.49E+26	-4.61	17253.	!	1.00E+00 a	tm, 60	0-2500 K,	98	err	::CM	:
PH + O2	<=> YOC6JDOA	3.17E+34	-6.75	25151.	!	1.00E+01 a	tm, 60	0-2500 K,	118	err	::CM	:
PH + O2	<=> YOC6JDOA	6.95E+36	-7.26	31429.	!	2.00E+02 a	tm, 60	0-2500 K,	16%	err	::CM	:
PH + O2	<=> PHOJ+O	4.09E+14	-0.32	1248.	1	1.00E-03 a	tm, 60	0-2500 K,	18	err	::CM	:
PH + O2	<=> PHOJ+O	4.22E+16	-0.87	2930.	!	1.00E-02 a	tm, 60	0-2500 K,	38	err	::CM	:
PH + O2	<=> PHOJ+O	6.21E+21	-2.29	7327.	1	1.00E-01 a	tm, 60	0-2500 K	9%	err	: : CM	:
PH + 02	<=> PHOJ+O	7.06E+29	-4.49	14560.	1	1.00E+00 a	.tm, 60	0-2500 K	15%	err	::CM	:
PH + 02	<=> PHOJ+O	1.40E+37	-6.44	22258.	1	1.00E+01 a	tm, 60	0-2500 K	15%	err	::CM	:
PH + 02	<=> PHOJ+O	4.29E+37	-6.42	27510.	1	2.00E+02 a	tm. 60	0-2500 K	17%	err	::CM	:
PH + O2	<=> C6JY00	2.83E+94	-29.85	20653.	i.	1.00E-03 a	.tm, 60	0-2500 K	42%	err	:: CM	:
PH + 02	<=> C6JY00	2.80+102	-31.49	28348.	1	1.00E-02 a	tm. 60	0-2500 K	428	err	:: CM	
PH + O2	$\leq = > C6JY00$	1.90+110	-33.11	36654	i	1 00E-01 a	tm. 60	0-2500 K	38%	err	: : C'M	÷
PH + O2	<=> C6JY00	1.08+115	-33.89	43428	i i	1 00E+00 a	tm. 60	0-2500 K	32%	err	: : CM	÷
PH + 02	$\leq = > C6 TY00$	1.20+113	-32.82	45766	1	1 00E+01 a	tm. 60	0-2500 K	45%	err	· · CM	÷
PH + 02	<=> C6JY00	3 44E+94	-27 05	37025	i	2 00E+02 a	tm. 60	0-2500 K	101%	err	::CM	
PH + 02	<=> YOC6JDO	5 69E+11	-6.02	4132	·	1 00E-03 a	tm, 60	0-2500 K	16%	err	• • CM	:
PH + 02		2 33E+16	-7 01	7127		1 00E-02 a	tm 60	0-2500 K	20%	err	• • CM	:
DH + 02		8 078-32	6 24	-35021	÷	1 00E-01 a	tm 60	0-2500 K	208	err	• • CM	:
DH + 02		4 458+68	-22 25	1519		1.00E+00 a	tm 60	0-2500 K	6988	err	• • CM	:
		4 16,102	E2 27	72051		1.005:01 3	tm 60	0 2500 K	5050 B	arr	CM	:
PH + 02		4.10+103	-53.27	/3051.	:	1.00E+01 a	.cm, 60	0-2500 K	117%	err	::CM	-
PH + 02		1.15+101	-50.16	09/01.	1	2.00E+02 a	1. L.III, 60	0-2500 K	1132	err	::CM	
PH + 02	<=> RODC6JD0	0.628+12	-0.17	-16//.	:	1.00E-03 a	.CM, 60	0-2500 K	55	err	::CM	:
PH + OZ	<=> RODC6JD0	3.70E+15	-0.92	615.	1	1.00E-02 a	Cm, 60	0-2500 K	, 87 150	err	::CM	:
PH + 02	<=> RODC6JDO	4.19E+21	-2.58	5787.	!	1.00E-01 a	.cm, 60	0-2500 K	158	err	::CM	:
PH + O2	<=> RODC6JDO	9.46E+29	-4.85	13401.	1	1.00E+00 a	.tm, 60	0-2500 K	218	err	::CM	:
PH + O2	<=> RODC6JDO	7.47E+36	-6.69	21002.	!	1.00E+01 a	tm, 60	0-2500 K	18%	err	::CM	:
PH + 02	<=> RODC6JDO	1.68E+43	-8.25	31871.	!	2.00E+02 a	.tm, 60	0-2500 K	168	err	::CM	:
PH + 02	<=> Y0C5J+C0	6.35E+07	0.43	1455.	!	1.00E-03 a	tm, 60	0-2500 K	, 5%	err	::CM	:
PH + 02	<=> YOC5J+CO	7.63E+09	-0.14	3189.	!	1.00E-02 a	tm, 60	0-2500 K	2%	err	::CM	:
PH + O2	<=> YOC5J+CO	1.23E+15	-1.57	7600.	1	1.00E-01 a	tm, 60	0-2500 K	48	err	::CM	:
PH + O2	<=> YOC5J+CO	2.17E+23	-3.82	14920.	ł	1.00E+00 a	.tm, 60	0-2500 K	, 10%	err	::CM	:
PH + O2	<=> YOC5J+CO	1.09E+32	-6.16	23658.	1	1.00E+01 a	.tm, 60	0-2500 K	, 12%	err	::CM	:
PH + O2	<=> YOC5J+CO	2.77E+40	-8.29	36087.	!	2.00E+02 a	tm, 60	0-2500 K	, 15%	err	::CM	:
PH + O2	<=> Y5JY04D0	1.19E+04	-4.66	4723.	!	1.00E-03 a	tm, 60	0-2500 K	, 31%	err	::CM	:

PH + 02	<=> Y5JY04D0		6.97E+07	-5.42	7027. 1	1.00E-02 atm.	600-2500 K.	33% err	::CM :
PH + O2	$\leq > X5 T X 04 D 0$		2.57E+14	-6.95	11778	1 00E-01 atm	600-2500 K	37% err	••CM •
PH + O2	$\leq > 15010100$		3 60E+23	-9.16	19178 1	1 00E+00 atm	600-2500 K	39% err	· . CM ·
PH + 02	$\leq > 150104D0$		3 07E-10	0.26	-7306	1 00E+01 atm	600-2500 K	54% err	••CM •
PH + 02			1 72E+72	-22 87	23182 1	2 00E+02 atm	600-2500 K	202% err	· · CM ·
PH + 02	<=> 13510400 <=> CY5.14CO2		9 48E+10	0 04	-292 (1 00E-03 atm	600-2500 K	0% err	· · CM ·
DH + 02	<=> CY5.1+CO2		2 48E+13	-0.62	1725 1	1 00E-02 atm	600-2500 K	3% err	· · · · · · · · · · · · · · · · · · ·
			1 118+10	-0.02	6523 1	1.00E-02 acm,	600-2500 K	98 err	CM .
PH + 02			2 408+27	-2.17	14029	1.00E+01 atm,	600-2500 K	15% err	
PH + 02			1 935+35	-6.56	22227	1.00E+00 acm,	600-2500 K	15% err	
PH + 02			3 408+40	-0.50	22237. 1	2.00E+01 atm,	600-2500 K,	15% err	
PH + 02			2 268-02	-3.37	2144 1	1.00E+02 atm,	600-2500 K,	15% err 45% err	
PH + 02			1 218.02	-3.13	5144. 1	1.00E-03 atm,	600-2500 K,	45% err	
$FH \neq 02$	VESOCODO		1.216+02	-3.88	10120	1.00E-02 acm,	600-2500 K,	403 EII	CM .
PH + OZ	<=> 105000D0		4.64E+08	-5.41	10138. !	1.00E-01 atm,	600-2500 K,	50% err	::CM :
PH + 02	<=> YC50CJD0		7.12E-48	10.12	-39445.	1.00E+00 atm,	600-2500 K,	/8% err	::CM :
PH + O2	<=> YC50CJD0		1.86E+27	-11.05	-11715. !	1.00E+01 atm,	600-2500 K,	330% err	::CM :
PH + OZ	<=> YC50CJD0		1.53+140	-41.66	58316. !	2.00E+02 atm,	600-2500 K,	20% err	::CM :
PH + O2	<=> CY5J+C02		3.778+08	0.36	2788. 1	1.00E-03 atm,	600-2500 K,	7∛ err	::CM :
PH + 02	<=> CY5J+C02		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+C02		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 + U2	4.31E+/2	-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, S%err	::CM :	
PHOOJ	<=> PHOJ+0	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	<=> C6JY00	1.78E+72	-17.92	72431.	! 1.00E-03	atm, 600-2500	K, 31% err	::CM :	
PHOOJ	<=> C6JY00	3.25E+73	-17.99	72775.	! 1.00E-02	atm, 600-2500	K, 31% err	::CM :	
PHOOJ	<=> C6JY00	1.19E+75	-18.13	74007.	! 1.00E-01	atm, 600-2500	K, 31% err	::CM :	
PHOOJ	<=> C6JY00	2.26E+76	-18.22	75906.	! 1.00E+00	atm, 600-2500	K, 31% err	::CM :	
PHOOJ	<=> C6JY00	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 :	
CEJYOO	<=> PHOOJ	3.80E+73	-18.29	73232.	! 1.00E-03	atm, 600-2500	K, 33% err	::CM :	
CEJYOO	<=> PHOOJ	3.80E+74	-18.29	73232.	! 1.00E-02	atm, 600-2500	K, 33% err	::CM :	
CEJYOO	<=> PHOOJ	3.80E+75	-18.29	73232.	! 1.00E-01	atm, 600-2500	K, 33% err	::CM :	
CEJYOO	<=> PHOOJ	3.82E+76	-18.29	73235.	! 1.00E+00	atm, 600-2500	K, 33% err	::CM :	
CEJYOO	<=> PHOOJ	3.99E+77	-18.29	73262.	! 1.00E+01	atm, 600-2500	K, 33% err	::CM :	

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CETVOO	2 m L		1 458179	-18 36	73681	1	2 008402	atm	600-2500 ¥	228	err	• • CM	
COLO	<->	YOCE IDO	1 150-73	-10.30	72021.	:	1 008-02	atm	600-2500 K,	228	orr	CM	:
CGTYOO	<=>	YOCE TOO	1 158-74	-10.32	73232.	:	1.00E-03	atm,	600-2500 K,	228	err	CM	
C60100	<=>	YOCE TOO	1 168-75	-10.32	73232.	:	1.00E-02	atm,	600-2500 K,	228	orr	<i>C</i> M	:
C60100	(-)	VOCETDO	1 158,76	-10.32	72222.	:	1.005-01	atm,	600-2500 K,	228	orr	CM	:
C6J100	<=>	YOCG TOO	1.156+70	-10.32	73235.	:	1.000+00	atill,	600-2500 K,	337 778	err	: CM	:
C6J100	<=>	YOCG TOO	1.206+77	-10.33	73201.	÷	1.006+01	atili,	600-2500 K,	ວວຈ ວວຍ	orr	::CM	:
C6J100	<=>	10C6JD0	4.415+/8	-18.40	/3683.	:	2.00E+02	atm,	600-2500 K,	338 078	err	::CM	:
YOCGJDO	<=>	RODCEJDO	3.446+34	-8.02	25970.	:	1.008-03	acm,	600-2500 K,	235	err	::CM	:
YOC6JDO	<=>	RODC6JDO	1.565+41	~9.65	30900.		1.008-02	acm,	600-2500 K,	298	err	::CM	:
YOCGJDO	<=>	RODCEJDO	8.446+4/	-11.22	37021.		1.00E-01	atm,	600-2500 K,	108	err	::CM	:
YOCGJDO	<=>	RODC6JDO	3.428+40	-8.71	35665.		1.008+00	acm,	600-2500 K,	18%	err	::CM	:
AOC PIDO	<=>	RODCGJDO	1.416+40	-8.30	3//91.	:	1.006+01	acm,	600-2500 K,	88	err	::CM	:
YOC6JDO	<=>	RODCEJDO	7.25E+30	-5.31	35175.	!	2.006+02	acm,	600-2500 K,	98	err	::CM	:
YOCEJDO	<=>	YOC5J+CO	1.67E+28	-10.81	36951.	1	1.00E-03	atm,	600-2500 K,	29%	err	::CM	:
YOCEJDO	<=>	YOC5J+CO	2.55E+48	-15.48	44477.	!	1.00E-02	atm,	600-2500 K,	42%	err	::CM	:
YOCEJDO	<=>	YOC5J+CO	2.96E+64	-18.72	56526.	1	1.00E-01	atm,	600-2500 K,	298	err	::CM	:
YOCEJDO	<≈>	YOC5J+CO	5.96E+58	-15.88	59310.	1	1.00E+00	atm,	600-2500 K,	34%	err	::CM	:
YOCEJDO	<≈>	YOC5J+CO	9.01E+64	-16.71	69146.	!	1.00E+01	atm,	600-2500 K,	238	err	::CM	:
YOC6JD0	<=>	YOC5J+CO	1.30E+52	-12.12	68985.	!	2.00E+02	atm,	600-2500 K,	14%	err	::CM	:
YOCEJDO	<=>	C6JY00	2.84E+09	-10.28	62648.	!	1.00E-03	atm,	600-2500 K,	29%	err	::CM	:
YOC6JDO	<=>	C6JY00	6.11E+26	-14.24	60827.	1	1.00E-02	atm,	600-2500 K,	43%	err	::CM	:
YOC6JDO	<=>	Cejxoo	3.72E+60	-22.20	68439.	1	1.00E-01	atm,	600-2500 K,	36%	err	::CM	:
YOC6JDO	<≈>	Cejyoo	4.38E+77	-24.36	80121.	!	1.00E+00	atm,	600-2500 K,	46%	err	::CM	:
YOC6JDO	<≈>	Cejioo	7.44E+92	-26.31	99751.	1	1.00E+01	atm,	600-2500 K,	388	err	::CM	:
YOC6JDO	<≈>	C6JYOO	6,48E+82	-21.31	108893.	1	2.00E+02	atm,	600-2500 K,	148	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	1.00E-02	atm,	600-2500 K,	378	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	1.00E+01	atm,	600-2500 K,	16%	err	::CM	:
YOC6JDO	<=>	¥5JYO4DO	1.88E+43	-9.10	53818.	1	2.00E+02	atm,	600-2500 K,	12%	err	::CM	:
Y5JY04D0	<=>	CY5J+CO2	3.20E+12	-1.78	5733.	1	1.00E-03	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	CY5J+CO2	3.23E+13	-1.79	5738.	!	1.00E-02	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	CY5J+CO2	3.49E+14	-1.79	5782.	1	1.00E-01	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	CY5J+CO2	5.78E+15	-1.85	6104.	!	1.00E+00	atm,	600-2500 K,	38	err	::CM	:
Y5JY04DO	<=>	CY5J+CO2	7.65E+16	-1.88	6917.	1	1.00E+01	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	CY5J+CO2	5.84E+20	-2.56	10845.	1	2.00E+02	atm,	600-2500 K,	88	err	::CM	:
Y5JY04D0	<=>	YOCEJDO	3.28E-02	-1.36	20997.	1	1.00E-03	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	YOC6JDO	2.95E-01	-1.35	20926.	!	1.00E-02	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	YOC6JDO	1.14E+00	-1.24	20264.	1	1.00E-01	atm,	600-2500 K,	3%	err	::CM	:
Y5JY04DO	<=>	YOC6JDO	3.08E-01	-0.83	16299.	1	1.00E+00	atm,	600-2500 K,	28	err	::CM	:
Y5JY04D0	<=>	YOC6JDO	2.73E+09	-3.20	13817.	!	1.00E+01	atm,	600-2500 K,	6%	err	::CM	:
Y5JY04D0	<=>	YOC6JDO	2.48E+34	-8.34	29394.	!	2.00E+02	atm,	600-2500 K,	24%	err	::CM	:
Y5JY04D0	<=>	YC50CJD0	1.18E-01	-1.40	21039.	ļ	1.00E-03	atm,	600-2500 K,	38	err	::CM	:
Y5JY04D0	<=>	YC50CJD0	1.06E+00	-1.39	20968.	1	1.00E-02	atm,	600-2500 K,	3%	err	::CM	:
Y5JY04D0	<=>	YC50CJD0	4.09E+00	-1.28	20305.	ļ	1.00E-01	atm.	600-2500 K.	3%	err	::CM	:
Y5JY04D0	<=>	YC50CJD0	1.10E+00	-0.87	16338	ļ	1.00E+00	atm.	600-2500 K.	2%	err	::CM	:
Y5JY04D0	<=>	YC50CJD0	8.90E+09	-3.23	13824		1.00E+01	atm.	600-2500 K.	6%	err	::CM	
Y5JY04D0	<=>	YC5OCJDO	1.51E+34	-8.18	28955	1	2.00E+02	atm.	600-2500 K.	23%	err	: : CM	:
YC50C TDO	<=>	CY5.T+CO2	8.918+29	-6 74	24845	1	1.00E-03	atm.	600-2500 K	18%	err	: . CM	
YC50CTDO	<=>	CY5J+CO2	8.998+30	-6 74	24850		1.00E-02	atm.	600-2500 K	18%	err	::CM	
YC50CTD0	<>	CY5.T+CO2	9 72E+31	-6 75	24899		1 00E-01	atm	600-2500 K	18%	err	··CM	:
10000000	~/	0100,001		0.75	2-000.	•	T.000 01	s c my	000 2000 M	TO 0			•

YC50CJD0	<=> CY5J+CO2	1.61E+33	-6.80	25257.	1	1.00E+00	atm,	600-2500 K,	19% err	::CM	:
YC50CJD0	<=> CY5J+CO2	1.02E+13	-0.47	16211.	!	1.00E+01	atm,	600-2500 K,	66% err	::CM	:
YCSOCJDO	<=> CY5J+CO2	2.45E+33	-6.05	28628.	!	2.00E+02	atm,	600-2500 K,	13% err	::CM	:
YC50CJD0	<=> Y5JY04D0	1.15E+31	-6.89	24827.	1	1.00E-03	atm,	600-2500 K,	18% err	::CM	;
YC50CJD0	<=> Y5JY04D0	1.16E+32	-6.89	24832.	!	1.00E-02	atm,	600-2500 K,	18% err	::CM	:
YC50CJD0	<=> Y5JY04D0	1.25E+33	-6.90	24882.	!	1.00E-01	atm,	600-2500 K,	19% err	::CM	:
YC50CJD0	<=> Y5JY04D0	1.90E+34	-6.95	25234.	1	1.00E+00	atm,	600-2500 K,	19% err	::CM	:
YC50CJD0	<=> Y5JY04D0	3.47E+15	-1.06	16853.	<u>1</u>	1.00E+01	atm,	600-2500 K,	59% err	::CM	:
YC50CJD0	<=> Y5JY04D0	2.67E+35	-6.58	28453.	1	2.00E+02	atm,	600-2500 K,	12% err	::CM	:

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