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1) Title Page

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Abstract: An improved chemical kinetic model for the toluene oxidation based on experimental data obtained in a premixed laminar low-pressure flame with vacuum ultraviolet (VUV) photoionization and molecular beam mass spectrometry (MBMS) techniques has been proposed. The present mechanism consists of 273 species up to chrysene and 1740 reactions. The rate constants of reactions of toluene, decomposition, reaction with oxygen, ipso-additions and metatheses with abstraction of phenylic H-atom are updated; new pathways of C_4 + C_2 species giving benzene and fulvene are added. Based on the experimental observations, combustion intermediates such as fulvenallene, naphtol, methylnaphthalene, acenaphthylene, 2-ethynylnaphthalene, phenanthrene, anthracene, 1-methylphenanthrene, pyrene and chrysene are involved in the present mechanism. The final toluene model leads to an overall satisfactory agreement between the experimentally observed and predicted mole fraction profiles for the major products and most combustion intermediates. The toluene depletion is governed by metathese giving benzyl radicals, ipso-addition forming benzene and metatheses leading to $C_6H_4CH_3$ radicals. A sensitivity analysis indicates that the unimolecular decomposition via the cleavage of a C-H bond has a strong inhibiting effect, while decomposition via C-C bond breaking, ipso-addition of H-atom to toluene, decomposition of benzyl radicals and

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reactions related to $C_6H_4CH_3$ radicals have promoting effect for the consumption of toluene. Moreover, flow rate analysis is performed to illustrate the formation pathways of mono- and polycyclic aromatics.

Keywords: Detailed kinetic modeling; Toluene; Premixed laminar flame; PAH.

1. Introduction

Aromatic compounds are major components of many practical fuels such as gasoline, diesel and jet fuels, and understanding their combustion kinetics is important in the design of efficient engines and in the abatement of atmospheric pollution [1]. Among the aromatic compounds, toluene is often the largest single aromatic component in gasoline and in premium gasoline the toluene mole fraction is as high as 35% [2]. In addition, toluene can be easily produced from the oxidation of other hydrocarbons and it serves as a key precursor leading to the formation of polyaromatic hydrocarbons (PAH) and soot. Therefore, the combustion chemistry of toluene is of great interest both because of toluene's toxicity [2], but also because toluene oxidation can lead to other toxic compounds.

Despite the great abundance of models concerning the oxidation of toluene [3-9], the lack of toluene flame data prevents the literature models to be validated under flame conditions. Therefore, the toluene degradation chemistry is not so well established under flame conditions and uncertainties still remain in the existing mechanisms. To our knowledge, only three studies were carried out on such purposes, by Linstedt and Maurice [5], El Bakali et al. [10] and Detilleux and Vandooren [11]. Recently, Li et al. [12] reported a detailed chemical structure of a fuel-rich toluene flame measured with molecular-beam mass spectrometry (MBMS) and tunable synchrotron VUV photoionization techniques. Many intermediates especially radicals and isomers that they identified were neither measured nor evaluated by models previously.

The objective of this work is to develop a comprehensive model for toluene oxidation under flame conditions, based on the newly reported flame data obtained by Li et al. [12]. The improved mechanism will provide a more complete model for toluene combustion. It could improve the understanding of the combustion of gasoline and jet fuels and of the formation of soot precursors which lead to pollutant emissions.

2. Chemical kinetic modeling

Simulations were performed using Chemkin Premix codes [13]. The kinetic scheme developed here is an extension of our mechanism of aromatic compounds combustion [9], the latest version of which has been recently validated using data obtained with a premixed flame containing indane [14]. Table 1 lists the modification and addition made to the latest model and the full mechanism is available as *supplementary material*.

The mechanism was updated in several aspects. The rate constants of the unimolecular (R1 and R2, see Table 1) and bimolecular initiations of toluene (R3) were replaced by values determined by Oehlschlaeger et al. [15,16]. The rate constants of two metatheses (R8 and R9) with abstraction of phenylic H-atom were renewed based on newly published data [21,22]. The kinetics of reactions of bibenzyl ($C_{14}H_{14}$) and related radicals (R11-R15) were taken from Sakai et al. [17]. The ipso-addition of OH to toluene, forming phenol and methyl radical (R7), was added with the kinetics reported by Seta et al. [18]. The metathesis reaction of toluene with CHO radical (R21) was considered with the rate constant proposed by Mehl et al. [19]. The new formation pathways of C_4 + C_2 giving benzene and fulvene proposed by Hansen et al. [20] were used (not shown in Table 1).

To reproduce the formation and consumption of large combustion intermediates, namely methylnaphthalene, acenaphthylene, 2-ethynylnaphthalene, phenanthrene, anthracene, 1-methylphenanthrene, pyrene and chrysene, which were not considered in our previous mechanism [14], reactions proposed by Slavinskaya et al. [21] have been added (not listed in Table 1). Moreover, two new species, fulvenallene ($C_5H_4CCH_2$) and naphtol have been considered based on the experimental observations. Their kinetic schemes are analogous to those of allene (R23-31) and phenol (R32-38), respectively.

The other key feature of the present model is the treatment of the rate constants of metatheses and ipso-addition of benzene and toluene, namely reactions R4-R6, R16 and R19. The rate constants of these five reactions were determined using theoretical calculations, which was performed with the CBS-QB3 method implemented in Gaussian03 [22]. Frequency analysis had made it possible to point out one imaginary frequency for each transition state (TS) with the mode of vibration corresponding to the reaction coordinate. Hindered rotors were taken into account and barrier heights have been calculated at the B3LYP/6-31G(d,p) level. Tunneling effect was considered for H-transfer from the relation given by Skodje and Truhlar [23]. The kinetic parameters were obtained from a fitting for several temperatures (400-2000 K), with a modified Arrhenius form. The rate constants of reactions R7 and R10 were adopted from similar reactions R16 and R19, respectively.

3. Results and discussion

3.1 Flame chemical structure

The detailed kinetic mechanism was tested by comparing simulated results with experiments performed by Li et al. [12]. The reported experimental temperature profile was used as input for simulations. To account for the perturbations induced by the quartz probe and the thermocouple [24], the temperature profile was shifted 2.5 mm away from the burner surface.

Figure 1 displays the mole fraction profiles of the major species (toluene, O_2, Ar, H_2, H_2O, CO, and CO_2), and a good agreement is observed between predicted and experimental results. Our model slightly underpredicts the production of CO and overpredicts the level of CO_2 in the post-flame zone. However, these differences are within the experimental error which was ±10% for major species, ±25% for intermediates with known photoionization cross sections and about a factor of two for those with estimated cross sections [12].

The mole fraction profiles of common combustion intermediates are shown in Figs. 2-4. Figure

2 presents the mole fraction profiles for species ≤C_3. Our mechanism makes fairly good predictions for the experimental concentrations of methane, ethylene, ketene (C_2H_2O), propyne (pC_3H_4) and allene (aC_3H_4) while it tends to overpredict the peak values of methyl and vinyl radicals. Although Li et al. [12] did not mention it, mass 42 could contain the contribution of propene (C_3H_6). The modeling result confirms that C_2H_2O is the dominant species and the contribution of C_3H_6 is negligible. The model captures well the shape of acetylene (C_2H_2) profile before its maximum value. However, the maximum concentration of C_2H_2 is underpredicted and a tail is observed further than 12.0 mm from the burner surface. A similar tail was exhibited for predicted C_2H_2 profile in modeling fuel-rich 1,3-butadiene flames by Hansen et al. [20]. For propargyl radical (C_3H_3), the mole fraction profile is fairly predicted according to experimental uncertainties.

Figure 3 summarizes the mole fraction profiles of C_4-C_7 and three oxygenated species. The predicted peak values of the two C_4H_4 isomers, vinylacetylene (vC_4H_4) and butatriene (tC_4H_4) reveals that vC_4H_4 is dominant for mass 52, which is in agreement with experimental observations. The modeled maximum concentration of 1,3-butadiene (1,3-C_4H_6) is located about 1.6 mm downstream compared to the corresponding experimental value, which could result from measurement uncertainties since the reaction path analysis identified the reaction of cyclopentadienyl radicals (C_5H_5#) with OH radicals to be the major formation route of 1,3-C_4H_6 and C_5H_5# is well predicted. Besides C_5H_5#, the model performs well at predicting the mole fraction profiles of benzene (C_6H_6#), phenyl (C_6H_5#), and benzyl radicals (C_7H_7). With the formation pathways proposed by Hansen et al. [20], fulvene (fC_6H_6) mole fraction is underpredicted by a factor of ten. The predicted mole fraction profile of fulvenallene, which is well reproduced in another low pressure fuel-rich toluene flame [11] using the present model (see Fig. S1 in *supplemental material*), is one-

fifth of the experimental one. However, the experimental error cannot be ruled out since the photoionization cross sections of fulvene and fulvenallene are estimated [12].

For the oxygenated species, the formation of benzylalcohol ($C_6H_5CH_2OH$) is fairly predicted while that of phenol (C_6H_5OH) tends to be underpredicted across the flame zone. However, measurement uncertainties cannot be ruled out, especially since both C_6H_5# and benzyl radicals, their major sources, are well captured by the present model. There is a big difference (3.8 mm) between the predicted and measured locations of the peak concentration of benzaldehyde (C_6H_5CHO). The experimental C_6H_5CHO profile is obtained by subtracting contributions of three C_8H_{10} species [12], a process that could introduce larger experimental error. Our mechanism makes fairly good reproduction of the mole fraction profiles including that of benzaldehyde in a CH_4/toluene doped flame [10] (see Figs. S2 and S3 in *supplemental material*), which gives some confidence in the model's predictions.

Figure 4 compares the predicted mole fraction profiles of C_8-C_{14} species with the measurements. The mono- and polycyclic aromatics such as indenyl radical (C_9H_7), naphthalene ($C_{10}H_8$) and phenanthrene ($pC_{14}H_{10}$) are predicted accurately and reasonable predictions are made for ethylbenzene (eC_8H_{10}) and methylnaphthalene ($C_{11}H_{10}$). Contributions from styrene (sC_8H_8) are underpredicted by a factor of more than two, which could be resulted from measurement uncertainties since the current model make good predictions for sC_8H_8 in both pure toluene [11] and CH_4/toluene [10] flames (see Figs. S1 and S3 in *supplemental material*). For mass 106, Li et al. assigned the threshold 8.47 eV to the ionization of *p*-xylene [12]. However, *o*-xylene (o-C_8H_{10}), which is an isomer and has close ionization energy to *p*-xylene (p-C_8H_{10}), could contribute to this threshold. The predicted peak concentration of *o*-xylene is five times larger than that of *p*-xylene and the experimental profile of C_8H_{10} compounds is fairly captured by that of *o*-xylene. Hence, *o*-xylene

is assigned as the dominant contributor to this threshold. For C_8H_9, the two isomers, 4-methylbenzyl (not considered in the model) and 1-phenylethyl (C_8H_9) radicals were not distinguished experimentally [12]. However, another isomer, *o*-methylbenzyl (o-C_8H_9) radical which has close ionization energy could also contribute to mass 105. The predicted o-C_8H_9 profile is in good agreement with the experimental C_8H_9 profile, indicating o-C_8H_9 is the dominant species. Three species, indane (C_9H_{10}), 2-ethynylphenol (not considered in the model) and benzofuran (C_8H_6O) were reported to contribute to mass 118 [12]. However, the predicted maximum mole fraction of indane (3.0×10^{-8}) is much smaller than the experimental peak value of mass 118 (6.6×10^{-5}). Since the indane mechanism made correct predication for indane and indene for both premixed flame and jet-stirred reactor results [14], we deem it more reasonable to attribute mass 118 to benzofuran (bC_8H_6O). For mass 144, it could contain the contribution of both 1,2,3,4-tetrahydro-1-methylene-naphthalene (not considered in the model) and naphtol ($C_{10}H_8O$).

3.2 Ways of toluene consumption

Figures 5 and 6 present sensitivity and flux analysis for the consumption of toluene at a temperature of 1510 K and 78.9% conversion. The sensitivity result displayed in Fig. 5 (C_0-C_2 reactions are not shown except for $O_2 + H = OH + O$ which has the most important promoting effect) indicates that the unimolecular decomposition via cleavage of C-H bond has a strong inhibiting effect on toluene consumption, while decomposition via C-C breaking, ipso-addition, decomposition of benzyl radicals and reactions related to $C_6H_4CH_3$ radicals have promoting effect. These results are consistent with the conclusion that the formation of benzyl and $C_6H_4CH_3$ radicals have respective inhibiting and promoting effect deduced from the results obtained in a jet-stirred reactor at 893 K [9].

As shown in Fig. 6, the major route of toluene consumption is metatheses by H, OH and CH_3 to produce the resonance-stabilized benzyl radicals. Besides reverse reaction to toluene, benzyl radicals

are mainly consumed through two pathways, thermal decomposition to C_2H_2 and C_5H_5# and addition of O-atom to give C_6H_5CHO. Benzyl radicals are also an important source of benzylalcohol by OH termination and ethylbenzene through combination with CH_3 radical. Moreover, benzyl radicals can decompose to C_5H_5CCH which further reacts yielding $C_5H_4CCH_2$.

Two less important channels, ipso-addition forming benzene and metatheses giving $C_6H_4CH_3$ radicals account for 11.6% and 11.2% of the toluene consumption, respectively. The flow rate analysis identifies the ipso-addition of H-atom as the major formation pathway of benzene. The importance of this reaction was confirmed by Dagaut et al. [8], El Bakali et al. [10] and Detilleux and Vandooren [11]. In a low-pressure CH_4/toluene flame, El Bakali et al. reported that toluene was mainly consumed by H-abstraction reactions with H and OH and by elimination of CH_3 [10], which is in good agreement with the conclusion given by Dagaut et al. [8] who studied the toluene oxidation in a jet-stirred reactor at 1 atm. Besides producing benzene and benzyl radical, Detilleux and Vandooren concluded that unimolecular decomposition yielding C_6H_5# and CH_3 radicals was another significant consumption channel for toluene combustion in rich conditions [11]. However, all the three groups did not pay attention to the role of $C_6H_4CH_3$ radicals. In our model, reaction of $C_6H_4CH_3$ radicals with oxygen molecule producing *ortho*-benzoquinone (OC_6H_4O) and CH_3 radicals plays a more significant role than the reaction C_6H_5# + O_2 = OC_6H_4O + H for the formation of OC_6H_4O which can decompose further to 2,4-cyclopentadien-1-one (C_5H_4O#) and finally to CO and C_4H_4. Besides OC_6H_4O, cresoxy radical ($OC_6H_4CH_3$) is another product of the reaction of $C_6H_4CH_3$ radicals with O_2. Da Silva et al. [1] studied the reaction pathways for $C_6H_4CH_3$ + O_2 systems and concluded that the dominant products were methyl-dioxo-hexadienyl radicals and $OC_6H_4CH_3$ + O. They proposed that *o*-quinone methide (*o*-QM) was a significant intermediate in toluene combustion [25]. However, *o*-QM was neither experimentally identified by Li et al. [12] nor reported by El

Bakali et al. [10]. In the present mechanism, *o*-QM was not included. In addition, $C_6H_4CH_3$ is an important source of *o*-xylene as mentioned above. Other minor pathways of toluene degradation are thermal decomposition giving C_6H_5# and CH_3, and ipso-addition of O-atom leading to the formation of $OC_6H_4CH_3$, most of which converts to C_6H_6#, C_2H_2, C_3H_3, aC_3H_4 and C_4H_4 by releasing CO.

3.3 Formation of mono-/polycyclic aromatics

Many mono- and polycyclic hydrocarbons such as benzene, phenylacetylene, styrene, ethylbenzene, indene, naphthalene, methylnaphthalene, phenanthrene, pyrene and chrysene, were experimentally observed in the toluene flame. Li et al. attributed the formation of many aromatic intermediates to the so-called HACA (hydrogen abstraction carbon addition) mechanism [12]. The formation routes of some aromatic species will be discussed from the present simulation results.

Benzene formation pathways were recently reviewed by Hansen et al. [26] and they concluded that the contributions of these channels were dependent on the fuel structure. In the current model, benzene formation is governed by the ipso-addition of H-atom to toluene, and the reaction $OC_6H_4CH_3 = C_6H_6\# + H + CO$, while in CH_4/toluene flame [10], the reaction $C_6H_5\# + H = C_6H_6\#$ was found to be more significant than the decomposition of $OC_6H_4CH_3$. According to the rate of production analysis, ethylbenzene is mainly formed via the radical combination of benzyl and CH_3 radicals. By H-abstraction, ethylbenzene can be converted to 1-phenylethyl radical. Most of styrene comes from the decomposition of 1-phenylethyl radical. The addition of OH to indenyl radicals which was the major source of styrene in indane flame [14] is also an important route for styrene production. The main reactions involved in the formation of phenylacetylene are (a) the decomposition of 1-phenylvinyl radical by breaking a C-H bond, (b) the ipso-addition of C_2H radical to benzene and (c) the addition of phenyl radical to C_2H_2.

All the reaction pathways of indene in this mechanism were adopted from [14]. The production

of indene occurs via the combination of H-atom and indenyl radical which comes from the reaction of C_4H_2 and C_5H_5#. Modeling shows that at low temperatures, naphthalene is mainly formed by the combination of benzyl and propargyl radicals, while at high temperatures (> 1000 K), the combination of cyclopentadienyl radicals is the major source. This is opposite to the conclusion obtained in non-premixed flame by McEnally and Pfefferle [27]. Based on theoretical calculation, Kislov and Mebel [28] proposed that pentafulvalene was the dominant product of C_5H_5# recombination at T > 1500 K and naphthalene was a minor product. However, the calculated ionization energy of pentafulvalene is 7.81 eV (B3LYP/6-311G(d,p), [22]) and only one threshold at 8.18eV was reported experimentally for mass 128 [12], indicating that scarce pentafulvalene is formed in the flame.

The formation of naphthyl from H-abstraction of naphthalene is an important route in the molecular growth process. The reactions of naphthyl with CH_3 radicals are responsible for the formation of methylnaphthalene. Phenanthrene ($C_{14}H_{10}$) production proceeds mostly through the reaction of naphthalene with C_4H_2 via HACA sequence. The major consumption routes of phenanthrene involve decomposition reactions leading to acenaphthylene and C_2H_2, isomerization to give anthracene, and O/OH addition to form ethynylnaphthalene. In addition to phenanthrene, the reactions of indenyl with propargyl radicals and of naphthalene with C_2H radicals exhibit noticeable contribution for the ethynylnaphthalene production. Moreover, pyrene and chrysene can be originated from the addition (via HACA sequence) of C_2H_2 to acenaphthylene, and of C_4H_2 to phenanthrene, respectively.

4. Conclusion

A detailed toluene combustion model has been developed by updating the oxidation kinetics of toluene and evaluating a low-pressure premixed laminar flame. The predictions by the present

mechanism are in reasonable agreement with the experimental results for both major products and combustion intermediates. On the basis of the predicted mole fraction profiles, some chemical structures are reassigned. The results indicate that toluene consumption mainly proceeds via the formation of benzene, benzyl, and $C_6H_4CH_3$ radicals. Benzene formation is governed by ipso-addition of H-atom to toluene and decomposition of $OC_6H_4CH_3$ radicals. At low temperature ($T < 1000$ K), naphthalene is mainly formed by the combination of benzyl and propargyl radicals, while at high temperature ($T > 1000$ K), combination of two cyclopentadienyl radicals is the major source of this biaromatic species. Furthermore, the key reaction pathways of other aromatics are identified by rate production analysis.

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Table 1 Modfied and added reactions used in the present study. $k = A\,T^n \exp(-Ea/RT)$, units are mol, s, cm^3 and kcal.

RN [a]	Reaction	A	*n*	E_a	Ref.
Modified reactions					
R1.	Toluene = benzyl + H	2.09E15	0.0	87.51	[15]
R2.	Toluene = C_6H_5# + CH_3	2.66E16	0.0	97.88	[15]
R3.	Toluene + O_2 = benzyl + HO_2	2.18E7	2.5	46.045	[16]
R4.	Toluene + H = C_6H_6# + CH_3	5.67E8	1.43	5.65	[b]
R5.	Toluene + H = benzyl + H_2	2.92E6	2.372	5.81	[b]
R6.	Toluene + CH_3 = benzyl + CH_4	3.91E0	3.76	6.98	[b]
R7.	Toluene + H = $C_6H_4CH_3$ + H_2	1.22E8	2.031	15.88	[c]
R8.	Toluene + OH = $C_6H_4CH_3$ + H_2O	1.36E4	2.7	0.6196	[18]
R9.	Toluene + HO_2 = $C_6H_4CH_3$ + H_2O_2	9.2E12	0.0	28.81	[17]
R10.	Toluene + CH_3 = $C_6H_4CH_3$ + CH_4	2.07E0	3.861	13.3	[c]
R11.	2Benzyl = bibenzyl	5.01E12	0.0	0.454	[17]
R12.	Bibenzyl = $C_{14}H_{13}$# + H	1.0E16	0.0	83.66	[17]
R13.	Bibenzyl + H = $C_{14}H_{13}$# + H_2	5.4E4	2.5	-1.9	[d]
R14.	Bibenzyl + benzyl = $C_{14}H_{13}$# + toluene	2.2E12	0.0	9.1	[17]
R15.	$C_{14}H_{13}$# = stilbene + H	7.94E15	0.0	51.864	[17]
R16.	C_6H_6# + H = C_6H_5# + H_2	1.22E8	2.031	15.88	[b]
R17.	C_6H_6# + OH = C_6H_5# + H_2O	1.36E4	2.7	0.6196	[18]
R18.	C_6H_6# + HO_2 = C_6H_5# + H_2O_2	9.2E12	0.0	28.81	[e]
R19.	C_6H_6# + CH_3 = C_6H_5# + CH_4	2.07E0	3.861	13.3	[b]
Added reactions					
R20.	Toluene + OH = C_6H_5OH# + CH_3	7.83E2	2.884	3.2193	[18]
R21.	Toluene + CHO = benzyl + HCHO	3.77E13	0.0	23.787	[19]
R22.	Benzyl = C_5H_5CCH + H	3.16E15	0.0	85.205	[5]
R23.	$C_6H_5C_2H_2$ + H = C_6H_5#C_2H + H_2	1.0E13	0.0	0.0	[5]
R24.	$C_6H_5C_2H_2$ + OH = C_6H_5#C_2H + H_2O	1.0E13	0.0	0.0	[5]
R25.	C_5H_5CCH = C_5H_5# + C_2H	4.2E15	0.0	125.0	[f]
R26.	C_5H_5CCH + H = C_5H_5# + C_2H_2	2.0E10	0.0	0.0	[5]
R27.	C_5H_5CCH + H = C_4H_4 + C_3H_3	6.0E10	0.0	0.0	[5]
R28.	C_5H_5CCH + OH = C_5H_5# + CH_2CO	4.3E11	0.0	-0.8	[f]
R29.	$C_5H_4CCH_2$ = C_5H_5CCH	2.5E12	0.0	59.0	[f]
R30.	$C_5H_4CCH_2$ + H = C_5H_5CCH + H	8.5E12	0.0	2.0	[f]
R31.	$C_5H_4CCH_2$ + OH = C_5H_5# + CH_2CO	2.0E12	0.0	-0.2	[f]
R32.	Naphthyl + OH = naphtol	1.0E13	0.0	0.0	[g]
R33.	Naphtol + H = naphtoxy + H_2	1.2E14	0.0	12.4	[g]
R34.	Naphtol + O = naphtoxy + OH	1.3E13	0.0	2.9	[g]
R35.	Naphtol + OH = naphtoxy + H_2O	1.4E8	1.4	-0.96	[g]
R36.	Naphtol + HO_2 = naphtoxy + H_2O_2	1.0E12	0.0	10.0	[g]
R37.	Naphtol + CH_3 = naphtoxy O + CH_4	1.8E11	0.0	7.7	[g]
R38.	Naphtoxy + H = naphtol	1.0E14	0.0	0.0	[g]

Note: [a] RN represents reaction number; [b] rate constants are calculated theoretically with CBS-QB3 method with Gaussian03 [22]; [c] rate constants taken equal to the values calculated theoretically with CBS-QB3 method with Gaussian03 [22] for similar reactions of benzene; [d] Rate constant estimated by using the correlations proposed by Heyberger et al. [29] in the case of alkenes; [e] rate constant taken equal to the value proposed for reaction R9; [f] rate constants estimated by analogy with the values for C_3H_4 (allene and propyne); [g] rate constants estimated by analogy with the values for phenol.

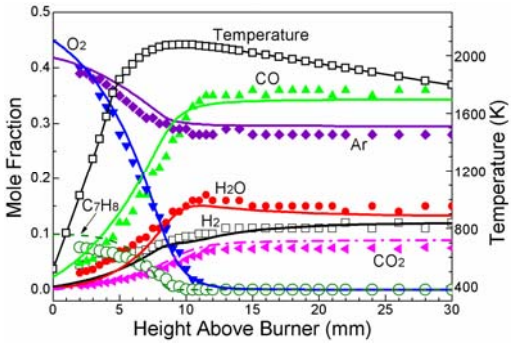

Fig. 1 Experimental (symbols) and predicted (lines) mole fraction profiles of major species toluene, O_2, Ar, H_2, H_2O, CO, and CO_2, along with the experimental temperature profile applied in the simulations.

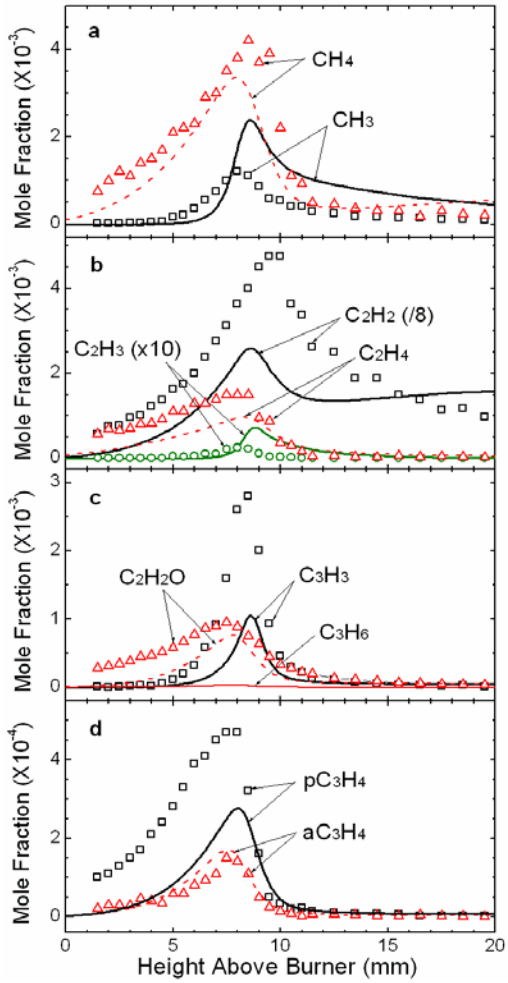

Fig. 2 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) CH_3 and CH_4; (b) C_2H_2, C_2H_3 and C_2H_4; (c) C_2H_2O (ketene), C_3H_3 (propargyl) and C_3H_6 (propene); (d) aC_3H_4 (allene) and pC_3H_4 (propyne).

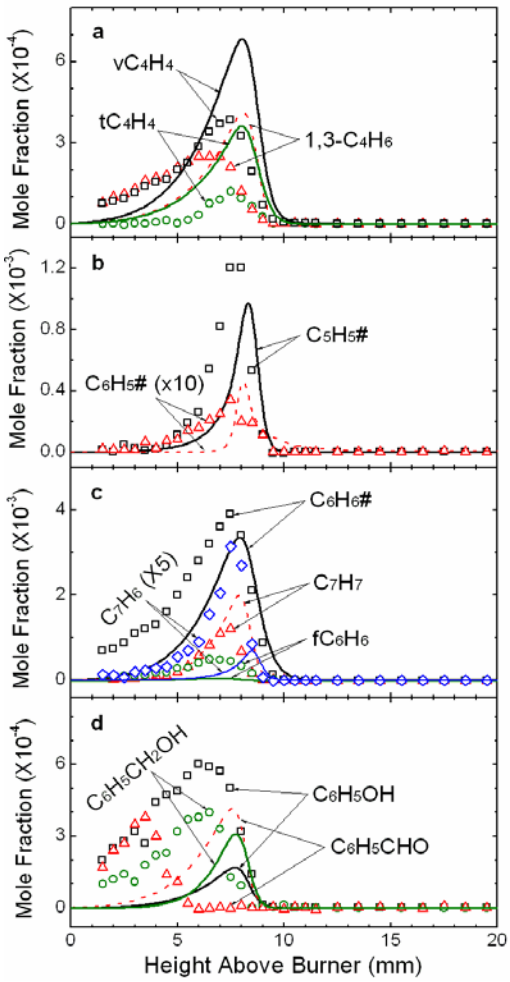

Fig. 3 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) vC_4H_4 (vinylacetylene), tC_4H_4 (butatriene) and 1,3-C_4H_6 (1,3-butadiene); (b) C_5H_5# (cyclopentadienyl) and C_6H_5# (phenyl); (c) C_6H_6# (benzene), fC_6H_6 (fulvene), $C_5H_4CCH_2$ (fulvenallene) and C_7H_7 (benzyl); (d) C_6H_5OH (phenol), C_6H_5CHO (benzaldehyde) and $C_6H_5CH_2OH$ (benzylalcohol).

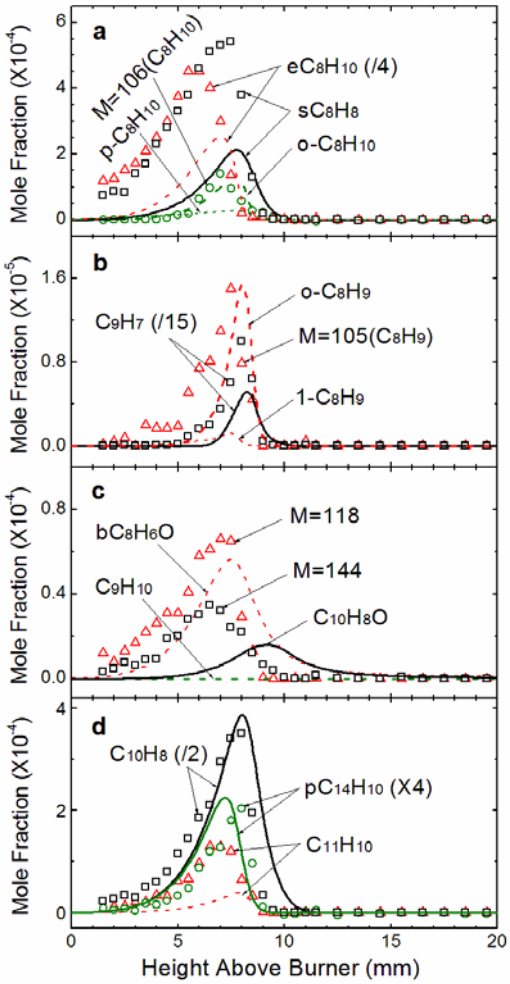

Fig. 4 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) sC_8H_8 (styrene), eC_8H_{10} (ethylbenzene), $o\text{-}C_8H_{10}$ (o-xylene) and $p\text{-}C_8H_{10}$ (p-xylene); (b) $1\text{-}C_8H_9$ (1-phenylethyl), $o\text{-}C_8H_9$ (o-methylbenzyl) and C_9H_7 (indenyl); (c) C_9H_{10} (indane), bC_8H_6O (benzofuran), and $C_{10}H_8O$ (naphtol); (d) $C_{10}H_8$ (naphthalene), $C_{11}H_{10}$ (methylnaphthalene) and $pC_{14}H_{10}$ (phenanthrene).

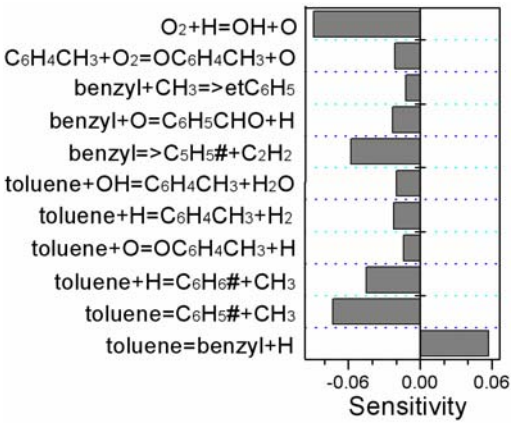

Fig. 5 Sensitivity analysis for the conversion of toluene at a distance of 7.8 mm from the burner, corresponding to temperature of 1510 K and 78.9% conversion of toluene.

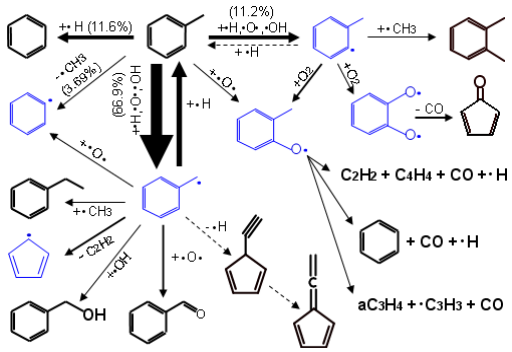

Fig. 6 Flow rate analysis for the consumption of toluene at a distance of 7.8 mm from the burner, corresponding to a temperature of 1510 K and a 78.9% conversion of toluene.

Figure captions

Color figure in electronic versions only

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Fig. 4 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) sC_8H_8 (styrene), eC_8H_{10} (ethylbenzene), o-C_8H_{10} (o-xylene) and p-C_8H_{10} (p-xylene); (b) 1-C_8H_9 (1-phenylethyl), o-C_8H_9 (o-methylbenzyl) and C_9H_7 (indenyl); (c) C_9H_{10} (indane), bC_8H_6O (benzofuran), and $C_{10}H_8O$ (naphtol); (d) $C_{10}H_8$ (naphthalene), $C_{11}H_{10}$ (methylnaphthalene) and $pC_{14}H_{10}$ (phenanthrene).

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Fig. 6 Flow rate analysis for the consumption of toluene at a distance of 7.8 mm from the burner, corresponding to a temperature of 1510 K and a 78.9% conversion of toluene.

List of Supplemental Material

A "supplemental material" is included in this paper. It consists of the following sections:

Section 1: **Simulated results for other toluene flame data**

Figure S1 is the experimental and predicted results of a low-pressure, fuel-rich toluene flame performed by Destilleux and Vandooren [*J. Phys. Chem. A 113 (2009) 10913-10922*]. Figures S2 and S3 are comparisons of the predictions by this work with the experimental results of CH_4/toluene flame performed by El Bakali et al. [*J. Phys. Chem. A 111 (2007) 3907-3921*].

Section 2: **List of species with known photoionization cross sections**

Combustion products and intermediates with known photoionization cross sections are listed.

Section 3: **The detailed reaction mechanism of this work**

The reaction mechanism developed in this study, including 273 species and 1740 reactions, is displayed in this section. The mechanism including the references for the kinetic parameters and the thermodynamic and transport databases are available from the authors at the following e-mail address: Zhenyu.Tian@ensic.inpl-nancy.fr.

Supplemental Material

Z.Y. Tian, W.J. Pitz, R. Fournet, P.A. Glaude, F. Battin-Leclerc, A detailed kinetic modeling study of toluene oxidation in a premixed laminar flame, *Proc. Combust. Inst.* 33, 2010.

Section 1: Simulated results for other toluene flame data

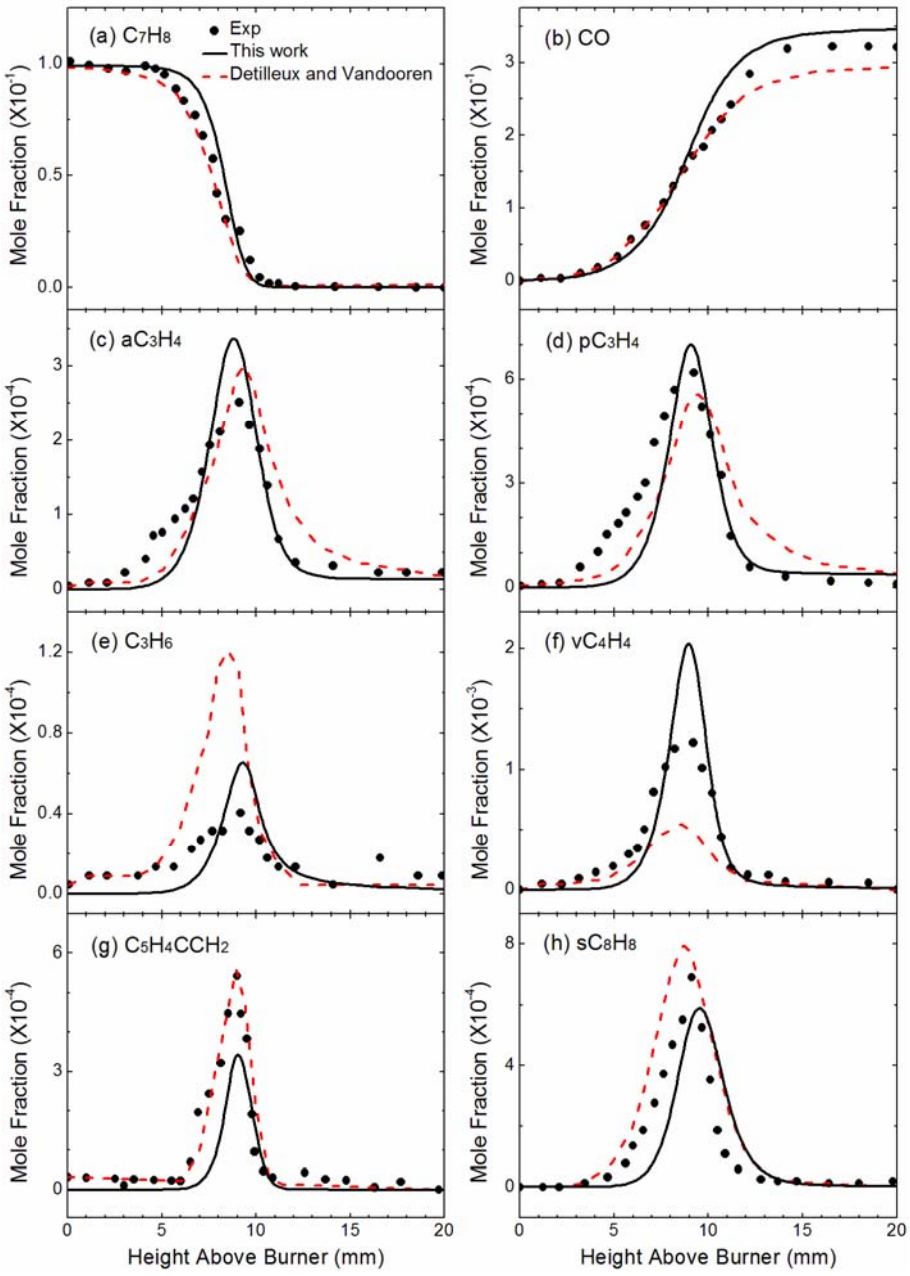

Fig. S1 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) C_7H_8 (toluene), (b) CO, (c) aC_3H_4 (allene), (d) pC_3H_4 (propyne), (e) C_3H_6 (propene), (f) vC_4H_4 (vinylacetylene), (g) $C_5H_4CCH_2$ (fulvenallene) and (h) sC_8H_8 (styrene) in a low-pressure, fuel-rich toluene flame performed by Detilleux and Vandooren [1]. Solid lines are predictions with the present mechanism and dashed lines are that with mechanism of Detilleux and Vandooren [1].

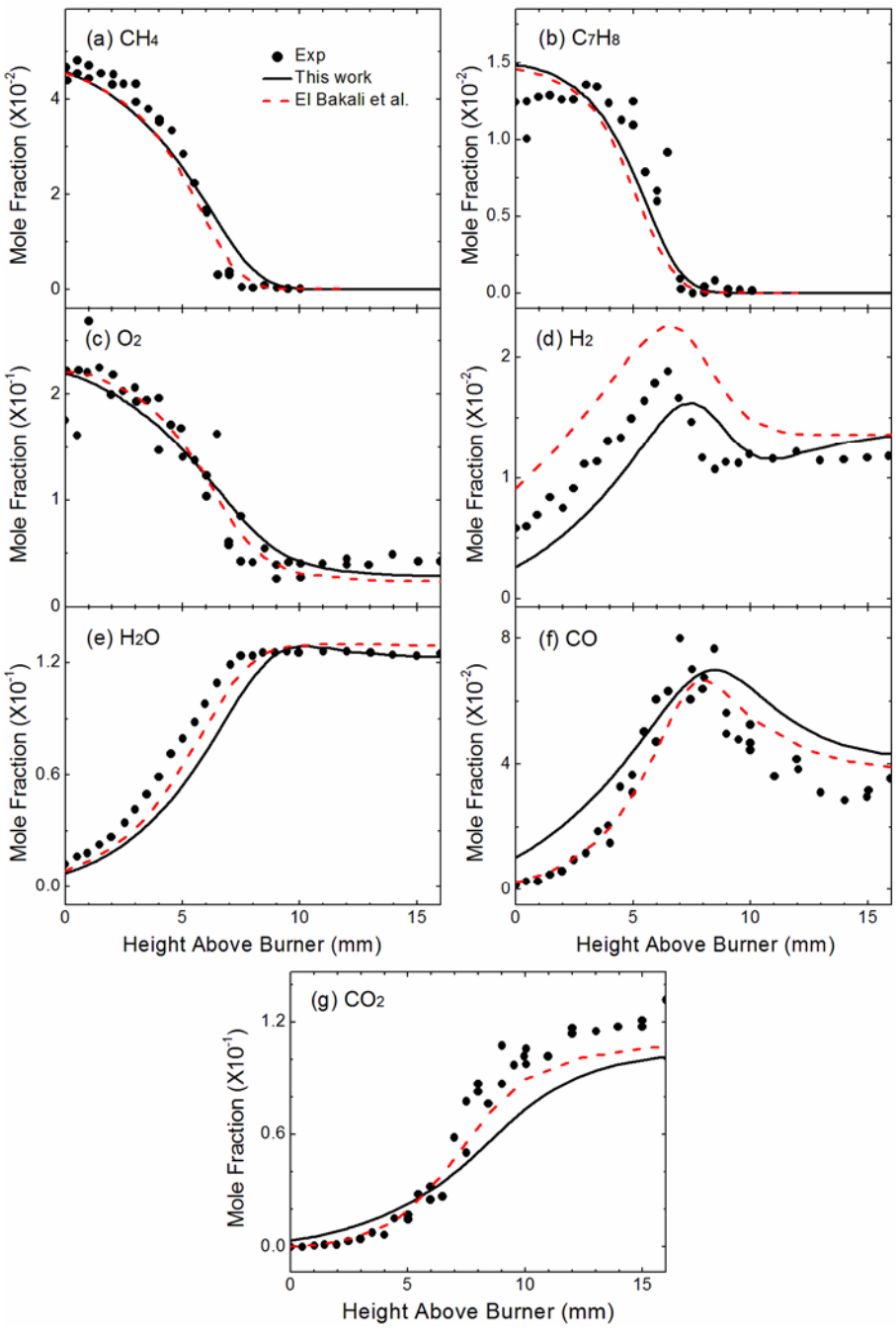

Fig. S2 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) CH_4, (b) C_7H_8 (toluene), (c) O_2, (d) H_2, (e) H_2O, (f) CO and (g) CO_2 in a low-pressure, stoichiometric CH_4/toluene flame performed by El Bakali et al.[2]. Solid lines are predictions with the present mechanism and dashed lines are that with mechanism of El Bakali et al. [2].

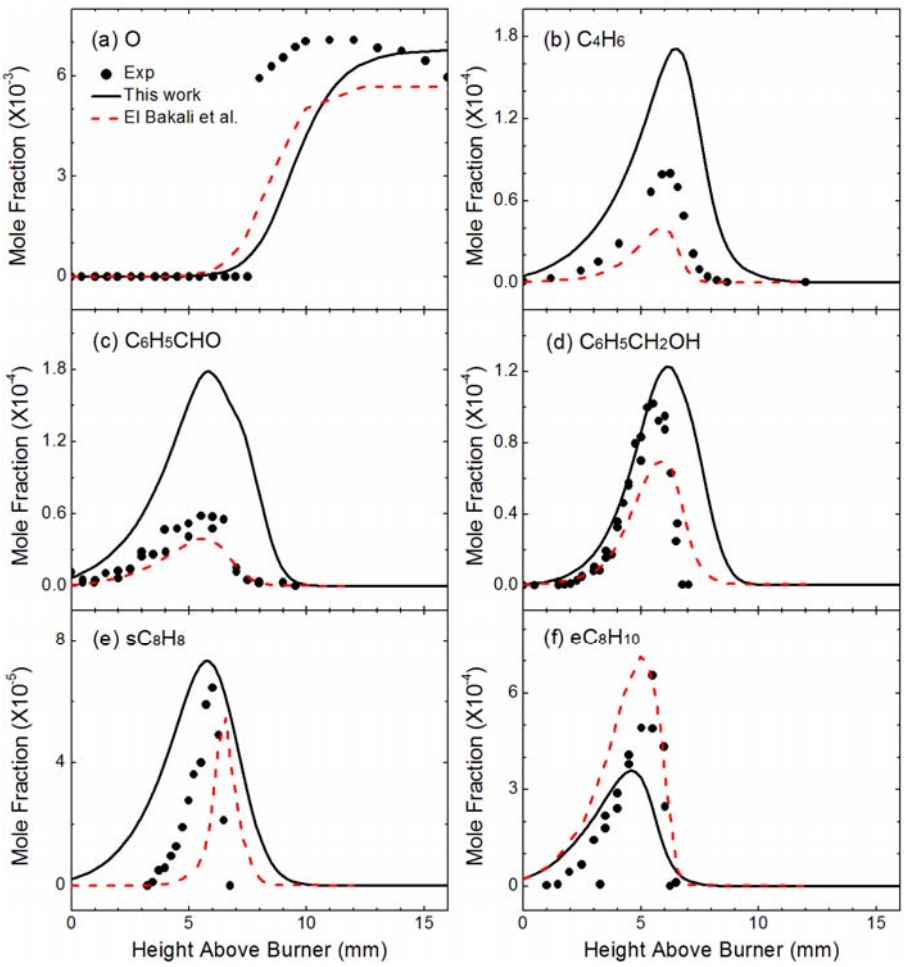

Fig. S3 Experimental (symbols) and predicted (lines) mole fraction profiles of (a) O, (b) C_4H_6 (1,3-butadiene), (c) C_6H_5CHO (benzaldehyde), (d) $C_6H_5CH_2OH$ (benzylalcohol), (e) sC_8H_8 (styrene) and (f) eC_8H_{10} (ethylbenzene) in a low-pressure, stoichiometric CH_4/toluene flame performed by El Bakali et al. [2]. Solid lines are predictions with the present mechanism and dashed lines are that with mechanism of El Bakali et al. [2].

Section 2: List of species with known photoionization cross sections [3-11]

H_2, O_2, CO, CO_2, CH_4, C_2H_2, C_2H_3, C_2H_4, HCHO, C_3H_3 (propargyl radical), aC_3H_4 (allene), pC_3H_4 (propyne), C_3H_5 (allyl radical), C_3H_6 (propene), vC_4H_4 (vinylacetylene), 1,3-C_4H_6 (1,3-butadiene) and C_6H_6# (benzene).

Section 3: The detailed reaction mechanism of this work

ELEMENTS CONSIDERED	ATOMIC WEIGHT
1. H	1.00797
2. O	15.9994
3. C	12.0112
4. N	14.0067
5. AR	39.9480
6. HE	4.00260
7. NE	20.1830

SPECIES CONSIDERED	PHASE	CHARGE	MOLECULAR WEIGHT	TEMPERATURE LOW	TEMPERATURE HIGH	ELEMENT COUNT H	O	C	N	AR	HE	NE
1. AR	G	0	39.94800	300.0	5000.0	0	0	0	0	1	0	0
2. N2	G	0	28.01340	300.0	5000.0	0	0	0	2	0	0	0
3. HE	G	0	4.00260	300.0	5000.0	0	0	0	0	0	1	0
4. NE	G	0	20.18300	300.0	5000.0	0	0	0	0	0	0	1
5. B1O	G	0	15.99940	300.0	5000.0	0	1	0	0	0	0	0
6. B2CO	G	0	28.01055	300.0	5000.0	0	1	1	0	0	0	0
7. B4CH	G	0	13.01912	300.0	5000.0	1	0	1	0	0	0	0
8. B5CH2	G	0	14.02709	300.0	5000.0	2	0	1	0	0	0	0
9. B6CH2	G	0	14.02709	300.0	5000.0	2	0	1	0	0	0	0
10. H2	G	0	2.01594	300.0	5000.0	2	0	0	0	0	0	0
11. H2O	G	0	18.01534	300.0	5000.0	2	1	0	0	0	0	0
12. O2	G	0	31.99880	300.0	5000.0	0	2	0	0	0	0	0
13. CH4	G	0	16.04303	300.0	5000.0	4	0	1	0	0	0	0
14. CO2	G	0	44.00995	300.0	5000.0	0	2	1	0	0	0	0
15. H2O2	G	0	34.01474	300.0	5000.0	2	2	0	0	0	0	0
16. HCHO	G	0	30.02649	300.0	5000.0	2	1	1	0	0	0	0
17. CH3OH	G	0	32.04243	300.0	5000.0	4	1	1	0	0	0	0
18. CH3OOH	G	0	48.04183	300.0	5000.0	4	2	1	0	0	0	0
19. C2H2	G	0	26.03824	300.0	5000.0	2	0	2	0	0	0	0
20. C2H4Z	G	0	28.05418	300.0	5000.0	4	0	2	0	0	0	0
21. C2H6	G	0	30.07012	300.0	5000.0	6	0	2	0	0	0	0

22. C2H4O#3	G	0	44.05358	300.0	5000.0	4	1	2	0	0	0	0
23. CH2COZ	G	0	42.03764	300.0	5000.0	2	1	2	0	0	0	0
24. CH3CHO	G	0	44.05358	300.0	5000.0	4	1	2	0	0	0	0
25. C2H5OH	G	0	46.06952	300.0	5000.0	6	1	2	0	0	0	0
26. C2H3CHO	G	0	56.06473	300.0	5000.0	4	1	3	0	0	0	0
27. C2H5CHO	G	0	58.08067	300.0	5000.0	6	1	3	0	0	0	0
28. C2H6CO	G	0	58.08067	300.0	5000.0	6	1	3	0	0	0	0
29. C3H2	G	0	38.04939	150.0	4000.0	2	0	3	0	0	0	0
30. cC3H4	G	0	40.06533	300.0	5000.0	4	0	3	0	0	0	0
31. aC3H4	G	0	40.06533	300.0	5000.0	4	0	3	0	0	0	0
32. pC3H4	G	0	40.06533	300.0	5000.0	4	0	3	0	0	0	0
33. C3H6Y	G	0	42.08127	300.0	5000.0	6	0	3	0	0	0	0
34. cC3H6	G	0	42.08127	300.0	5000.0	6	0	3	0	0	0	0
35. C3H8	G	0	44.09721	300.0	5000.0	8	0	3	0	0	0	0
36. C4H2	G	0	50.06054	300.0	5000.0	2	0	4	0	0	0	0
37. C4H4	G	0	52.07648	300.0	5000.0	4	0	4	0	0	0	0
38. tC4H4	G	0	52.07648	300.0	5000.0	4	0	4	0	0	0	0
39. C4H6Z2	G	0	54.09242	300.0	5000.0	6	0	4	0	0	0	0
40. C4H6-12	G	0	54.09242	300.0	5000.0	6	0	4	0	0	0	0
41. cC4H6	G	0	54.09242	300.0	5000.0	6	0	4	0	0	0	0
42. C4H6-1	G	0	54.09242	300.0	5000.0	6	0	4	0	0	0	0
43. C4H6-2	G	0	54.09242	300.0	5000.0	6	0	4	0	0	0	0
44. C4H8Y	G	0	56.10836	300.0	5000.0	8	0	4	0	0	0	0
45. iC4H8	G	0	56.10836	300.0	5000.0	8	0	4	0	0	0	0
46. C4H10	G	0	58.12430	300.0	5000.0	10	0	4	0	0	0	0
47. C5H4O#	G	0	80.08703	300.0	5000.0	4	1	5	0	0	0	0
48. C5H8	G	0	68.11951	300.0	5000.0	8	0	5	0	0	0	0
49. iC5H8	G	0	68.11951	300.0	5000.0	8	0	5	0	0	0	0
50. iC5H10	G	0	70.13545	300.0	5000.0	10	0	5	0	0	0	0
51. C5H10	G	0	70.13545	300.0	5000.0	10	0	5	0	0	0	0
52. C5H8#	G	0	68.11951	300.0	5000.0	8	0	5	0	0	0	0
53. C5H6#	G	0	66.10357	300.0	5000.0	6	0	5	0	0	0	0
54. C6H2	G	0	74.08284	300.0	5000.0	2	0	6	0	0	0	0
55. lC6H4	G	0	76.09878	300.0	5000.0	4	0	6	0	0	0	0
56. lC6H6	G	0	78.11472	300.0	5000.0	6	0	6	0	0	0	0
57. C6H6#	G	0	78.11472	300.0	5000.0	6	0	6	0	0	0	0
58. lC6H8	G	0	80.13066	300.0	5000.0	8	0	6	0	0	0	0
59. C6H8#	G	0	80.13066	300.0	5000.0	8	0	6	0	0	0	0
60. C6H10#	G	0	82.14660	300.0	5000.0	10	0	6	0	0	0	0
61. C6H10Y	G	0	82.14660	300.0	5000.0	10	0	6	0	0	0	0
62. toluene	G	0	92.14181	300.0	5000.0	8	0	7	0	0	0	0
63. MCP	G	0	82.14660	300.0	5000.0	10	0	6	0	0	0	0

64. MCPD	G	0	80.13066	300.0	5000.0	8	0	6	0	0	0	0
65. C8H10#	G	0	106.16890	300.0	5000.0	10	0	8	0	0	0	0
66. R1H	G	0	1.00797	300.0	5000.0	1	0	0	0	0	0	0
67. R2OH	G	0	17.00737	300.0	5000.0	1	1	0	0	0	0	0
68. R3OOH	G	0	33.00677	300.0	5000.0	1	2	0	0	0	0	0
69. R4CH3	G	0	15.03506	300.0	5000.0	3	0	1	0	0	0	0
70. R5CHO	G	0	29.01852	300.0	5000.0	1	1	1	0	0	0	0
71. R6CH2OH	G	0	31.03446	300.0	5000.0	3	1	1	0	0	0	0
72. R7CH3O	G	0	31.03446	300.0	5000.0	3	1	1	0	0	0	0
73. R8CH3OO	G	0	47.03386	300.0	5000.0	3	2	1	0	0	0	0
74. R9C2H	G	0	25.03027	300.0	5000.0	1	0	2	0	0	0	0
75. R10C2H3V	G	0	27.04621	300.0	5000.0	3	0	2	0	0	0	0
76. R11C2H5	G	0	29.06215	300.0	5000.0	5	0	2	0	0	0	0
77. R12CHCOZ	G	0	41.02967	300.0	5000.0	1	1	2	0	0	0	0
78. R13CH2CHO	G	0	43.04561	300.0	5000.0	3	1	2	0	0	0	0
79. R14CH3CO	G	0	43.04561	300.0	5000.0	3	1	2	0	0	0	0
80. R15C2H5O	G	0	45.06155	300.0	5000.0	5	1	2	0	0	0	0
81. R19C3H7	G	0	43.08924	300.0	5000.0	7	0	3	0	0	0	0
82. R20C4H9	G	0	57.11633	300.0	5000.0	9	0	4	0	0	0	0
83. iC3H7	G	0	43.08924	300.0	5000.0	7	0	3	0	0	0	0
84. nC3H7	G	0	43.08924	300.0	5000.0	7	0	3	0	0	0	0
85. C3H3	G	0	39.05736	300.0	5000.0	3	0	3	0	0	0	0
86. C3H5Y	G	0	41.07330	300.0	4000.0	5	0	3	0	0	0	0
87. tC3H5	G	0	41.07330	300.0	4000.0	5	0	3	0	0	0	0
88. sC3H5	G	0	41.07330	300.0	4000.0	5	0	3	0	0	0	0
89. nC4H3	G	0	51.06851	300.0	5000.0	3	0	4	0	0	0	0
90. iC4H3	G	0	51.06851	300.0	5000.0	3	0	4	0	0	0	0
91. nC4H5	G	0	53.08445	300.0	5000.0	5	0	4	0	0	0	0
92. iC4H5	G	0	53.08445	300.0	5000.0	5	0	4	0	0	0	0
93. C4H5-1s	G	0	53.08445	300.0	5000.0	5	0	4	0	0	0	0
94. C4H5-1p	G	0	53.08445	300.0	5000.0	5	0	4	0	0	0	0
95. C4H5-2	G	0	53.08445	300.0	5000.0	5	0	4	0	0	0	0
96. lC6H5	G	0	77.10675	300.0	5000.0	5	0	6	0	0	0	0
97. lC6H7	G	0	79.12269	300.0	5000.0	7	0	6	0	0	0	0
98. lC6H9	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
99. C6H4#	G	0	76.09878	300.0	5000.0	4	0	6	0	0	0	0
100. C6H5#	G	0	77.10675	300.0	5000.0	5	0	6	0	0	0	0
101. C6H7#	G	0	79.12269	300.0	5000.0	7	0	6	0	0	0	0
102. C6H9Z#	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
103. C4H7-1	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0
104. C4H7-2	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0
105. C4H7Y	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0

106. C4H7T	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0
107. iC4H7	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0
108. C4H7V	G	0	55.10039	300.0	5000.0	7	0	4	0	0	0	0
109. C5H7Y	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
110. iC5H7Y	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
111. C5H9Y	G	0	69.12748	300.0	5000.0	9	0	5	0	0	0	0
112. iC5H9	G	0	69.12748	300.0	5000.0	9	0	5	0	0	0	0
113. iC5H9Y	G	0	69.12748	300.0	5000.0	9	0	5	0	0	0	0
114. CH2CHCO	G	0	55.05676	300.0	5000.0	3	1	3	0	0	0	0
115. cC3H3	G	0	39.05736	300.0	5000.0	3	0	3	0	0	0	0
116. C4H4O	G	0	68.07588	300.0	5000.0	4	1	4	0	0	0	0
117. lC5H6	G	0	66.10357	300.0	5000.0	6	0	5	0	0	0	0
118. C5H5OH#	G	0	82.10297	300.0	5000.0	6	1	5	0	0	0	0
119. C6H5OH#	G	0	94.11412	300.0	5000.0	6	1	6	0	0	0	0
120. OC6H4O	G	0	108.09758	300.0	5000.0	4	2	6	0	0	0	0
121. C6H5#C2H	G	0	102.13702	300.0	5000.0	6	0	8	0	0	0	0
122. etC6H5	G	0	106.16890	300.0	5000.0	10	0	8	0	0	0	0
123. styrene	G	0	104.15296	300.0	5000.0	8	0	8	0	0	0	0
124. C6H5C3H3	G	0	116.16411	300.0	5000.0	8	0	9	0	0	0	0
125. methylindene	G	0	130.19120	300.0	5000.0	10	0	10	0	0	0	0
126. C6H5CHO	G	0	106.12527	300.0	5000.0	6	1	7	0	0	0	0
127. biphenyl	G	0	154.21350	300.0	5000.0	10	0	12	0	0	0	0
128. C5H5#	G	0	65.09560	300.0	5000.0	5	0	5	0	0	0	0
129. lC5H5	G	0	65.09560	300.0	5000.0	5	0	5	0	0	0	0
130. C5H3O#	G	0	79.07906	300.0	5000.0	3	1	5	0	0	0	0
131. C5H5O#	G	0	81.09500	300.0	5000.0	5	1	5	0	0	0	0
132. C5H4OH#	G	0	81.09500	300.0	5000.0	5	1	5	0	0	0	0
133. C6H5O#	G	0	93.10615	300.0	5000.0	5	1	6	0	0	0	0
134. C6H5O2	G	0	109.10555	300.0	5000.0	5	2	6	0	0	0	0
135. C6H4OH#	G	0	93.10615	300.0	5000.0	5	1	6	0	0	0	0
136. OC6H4OH	G	0	109.10555	300.0	5000.0	5	2	6	0	0	0	0
137. naphthalene	G	0	128.17526	200.0	6000.0	8	0	10	0	0	0	0
138. fulvene	G	0	78.11472	300.0	3000.0	6	0	6	0	0	0	0
139. HOC6H4CH3	G	0	108.14121	300.0	5000.0	8	1	7	0	0	0	0
140. C6H4OHCHO	G	0	122.12467	300.0	5000.0	6	2	7	0	0	0	0
141. C6H5CH2OH	G	0	108.14121	300.0	5000.0	8	1	7	0	0	0	0
142. C6H4CH3CHO	G	0	120.15236	300.0	5000.0	8	1	8	0	0	0	0
143. bibenzyl	G	0	182.26768	300.0	5000.0	14	0	14	0	0	0	0
144. stilbene	G	0	180.25174	300.0	5000.0	12	0	14	0	0	0	0
145. benzyl	G	0	91.13384	300.0	5000.0	7	0	7	0	0	0	0
146. C6H4CH3	G	0	91.13384	300.0	5000.0	7	0	7	0	0	0	0
147. OC6H4CHO	G	0	121.11670	300.0	5000.0	5	2	7	0	0	0	0

148. C6H4OHCO	G	0	121.11670	300.0	5000.0	5	2	7	0	0	0	0
149. HOC6H4CH2OO	G	0	139.13204	300.0	5000.0	7	3	7	0	0	0	0
150. OC6H4CH3	G	0	107.13324	300.0	5000.0	7	1	7	0	0	0	0
151. HOC6H4CH2	G	0	107.13324	300.0	5000.0	7	1	7	0	0	0	0
152. C6H5CO	G	0	105.11730	300.0	5000.0	5	1	7	0	0	0	0
153. C6H5CHOH	G	0	107.13324	300.0	5000.0	7	1	7	0	0	0	0
154. C6H5CH2O	G	0	107.13324	300.0	5000.0	7	1	7	0	0	0	0
155. HOC6H4CH2O	G	0	123.13264	300.0	5000.0	7	2	7	0	0	0	0
156. C8H9#	G	0	105.16093	300.0	5000.0	9	0	8	0	0	0	0
157. C8H9#-1	G	0	105.16093	300.0	5000.0	9	0	8	0	0	0	0
158. etC6H4	G	0	105.16093	300.0	5000.0	9	0	8	0	0	0	0
159. etC6H4O	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
160. C6H5C2H2	G	0	103.14499	300.0	5000.0	7	0	8	0	0	0	0
161. C14H13#	G	0	181.25971	300.0	5000.0	13	0	14	0	0	0	0
162. etC6H4OH	G	0	122.16830	300.0	5000.0	10	1	8	0	0	0	0
163. A2C2H	G	0	152.19756	200.0	6000.0	8	0	12	0	0	0	0
164. A2CH3	G	0	142.20235	200.0	6000.0	10	0	11	0	0	0	0
165. A2CH2	G	0	141.19438	200.0	6000.0	9	0	11	0	0	0	0
166. phenanthrene	G	0	178.23580	200.0	6000.0	10	0	14	0	0	0	0
167. pyrene	G	0	202.25811	200.0	6000.0	10	0	16	0	0	0	0
168. CH3phenanth	G	0	192.26290	300.0	5000.0	12	0	15	0	0	0	0
169. CH2phenanth	G	0	191.25493	300.0	5000.0	11	0	15	0	0	0	0
170. A2R5	G	0	152.19756	300.0	5000.0	8	0	12	0	0	0	0
171. naphtol	G	0	144.17466	300.0	5000.0	8	1	10	0	0	0	0
172. A2O	G	0	143.16669	300.0	5000.0	7	1	10	0	0	0	0
173. C5H4CCH2	G	0	90.12587	300.0	5000.0	6	0	7	0	0	0	0
174. C5H5CCH	G	0	90.12587	300.0	5000.0	6	0	7	0	0	0	0
175. chrysene	G	0	228.29635	300.0	5000.0	12	0	18	0	0	0	0
176. antra	G	0	178.23580	300.0	5000.0	10	0	14	0	0	0	0
177. o-xylene	G	0	106.16890	300.0	5000.0	10	0	8	0	0	0	0
178. o-methylbenzyl	G	0	105.16093	300.0	5000.0	9	0	8	0	0	0	0
179. phenyl(CH3)2	G	0	105.16093	300.0	5000.0	9	0	8	0	0	0	0
180. CH3C6H3OHCO	G	0	135.14379	300.0	5000.0	7	2	8	0	0	0	0
181. OC6H3(CH3)2	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
182. CH3HOC6H3CH2	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
183. CH3C6H4CO	G	0	119.14439	300.0	5000.0	7	1	8	0	0	0	0
184. CH3C6H4CHOH	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
185. CH3C6H4CH2O	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
186. CH3HOC6H3CH2O	G	0	137.15973	300.0	5000.0	9	2	8	0	0	0	0
187. CH3C6H4CH2OO	G	0	137.15973	300.0	5000.0	9	2	8	0	0	0	0
188. CH3C6H4CHCH3	G	0	119.18802	300.0	5000.0	11	0	9	0	0	0	0
189. o-C14H13#	G	0	209.31390	300.0	5000.0	17	0	16	0	0	0	0

190. HOC6H3(CH3)2	G	0	122.16830	300.0	5000.0	10	1	8	0	0	0	0
191. CH3OHC6H3CHO	G	0	136.15176	300.0	5000.0	8	2	8	0	0	0	0
192. CH3C6H4CH2OH	G	0	122.16830	300.0	5000.0	10	1	8	0	0	0	0
193. CH3C6H4CH2OOH	G	0	138.16770	300.0	5000.0	10	2	8	0	0	0	0
194. o-bibenzyl	G	0	210.32187	300.0	5000.0	18	0	16	0	0	0	0
195. o-stilbene	G	0	208.30593	300.0	5000.0	16	0	16	0	0	0	0
196. CH3C6H4CH2CH3	G	0	120.19599	300.0	5000.0	12	0	9	0	0	0	0
197. trimetbenz	G	0	120.19599	300.0	5000.0	12	0	9	0	0	0	0
198. CH3C6H4CHO	G	0	120.15236	300.0	5000.0	8	1	8	0	0	0	0
199. benzylCH2OH	G	0	121.16033	300.0	5000.0	9	1	8	0	0	0	0
200. CH3C6H4OH#	G	0	107.13324	300.0	5000.0	7	1	7	0	0	0	0
201. CH3styre	G	0	118.18005	300.0	5000.0	10	0	9	0	0	0	0
202. C10H10	G	0	130.19120	300.0	5000.0	10	0	10	0	0	0	0
203. o-xylylene	G	0	104.15296	300.0	5000.0	8	0	8	0	0	0	0
204. benzocyclobut	G	0	104.15296	300.0	5000.0	8	0	8	0	0	0	0
205. C10H9	G	0	129.18323	300.0	5000.0	9	0	10	0	0	0	0
206. bibibenzyl	G	0	196.29478	300.0	5000.0	16	0	15	0	0	0	0
207. CH2OC6H4CHO	G	0	135.14379	300.0	5000.0	7	2	8	0	0	0	0
208. C6H4CHO	G	0	105.11730	300.0	5000.0	5	1	7	0	0	0	0
209. CH2C6H4CHO	G	0	119.14439	300.0	5000.0	7	1	8	0	0	0	0
210. o-phtaldehyde	G	0	134.13582	300.0	5000.0	6	2	8	0	0	0	0
211. C5H8-12	G	0	68.11951	300.0	5000.0	8	0	5	0	0	0	0
212. C5H7#	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
213. C5H7#Y	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
214. C5H7#V	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
215. C5H7-1s	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
216. C5H7-2s	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
217. C5H7-4s	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
218. C5H7-3t	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
219. C5H7-5p	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
220. C5H7-12-5p	G	0	67.11154	300.0	5000.0	7	0	5	0	0	0	0
221. C5H9#	G	0	69.12748	300.0	5000.0	9	0	5	0	0	0	0
222. C5H9	G	0	69.12748	300.0	5000.0	9	0	5	0	0	0	0
223. RMCP1	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
224. RMCP2	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
225. RMCPY1	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
226. RMCPY2	G	0	81.13863	300.0	5000.0	9	0	6	0	0	0	0
227. RMCPD	G	0	79.12269	300.0	5000.0	7	0	6	0	0	0	0
228. RMCPDY	G	0	79.12269	300.0	5000.0	7	0	6	0	0	0	0
229. indane	G	0	118.18005	300.0	5000.0	10	0	9	0	0	0	0
230. indene	G	0	116.16411	300.0	5000.0	8	0	9	0	0	0	0
231. benzofuran	G	0	118.13642	200.0	6000.0	6	1	8	0	0	0	0

232. ph#C3H5Z	G	0	118.18005	300.0	5000.0	10	0	9	0	0	0	0
233. ph#C3H5p	G	0	118.18005	300.0	5000.0	10	0	9	0	0	0	0
234. ph#C3H7	G	0	120.19599	300.0	5000.0	12	0	9	0	0	0	0
235. ph#C4H9	G	0	134.22308	300.0	5000.0	14	0	10	0	0	0	0
236. cumene	G	0	120.19599	300.0	5000.0	12	0	9	0	0	0	0
237. anisole	G	0	108.14121	300.0	5000.0	8	1	7	0	0	0	0
238. C2H3C6H4CHO	G	0	132.16351	300.0	5000.0	8	1	9	0	0	0	0
239. C9H8O#	G	0	132.16351	300.0	5000.0	8	1	9	0	0	0	0
240. methylindane	G	0	132.20714	300.0	5000.0	12	0	10	0	0	0	0
241. C9H6O#	G	0	130.14757	300.0	5000.0	6	1	9	0	0	0	0
242. C8H8O#	G	0	120.15236	300.0	5000.0	8	1	8	0	0	0	0
243. C3H5C6H4CH3	G	0	132.20714	300.0	5000.0	12	0	10	0	0	0	0
244. methylindene-2	G	0	130.19120	300.0	5000.0	10	0	10	0	0	0	0
245. ph#C4H7-3	G	0	132.20714	300.0	5000.0	12	0	10	0	0	0	0
246. indanyl-Y	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
247. indanyl-1	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
248. C2H3C6H4CH2	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
249. C3H5C6H4	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
250. CH3C6H4C3H6	G	0	133.21511	300.0	5000.0	13	0	10	0	0	0	0
251. C9H9O#	G	0	133.17148	300.0	5000.0	9	1	9	0	0	0	0
252. C2H3C6H4CH2O	G	0	133.17148	300.0	5000.0	9	1	9	0	0	0	0
253. C3H5C6H4O	G	0	133.17148	300.0	5000.0	9	1	9	0	0	0	0
254. C9H7O#	G	0	131.15554	300.0	5000.0	7	1	9	0	0	0	0
255. ph#C3H6-1	G	0	119.18802	300.0	5000.0	11	0	9	0	0	0	0
256. ph#C3H6-2	G	0	119.18802	300.0	5000.0	11	0	9	0	0	0	0
257. ph#C3H6-Y	G	0	119.18802	300.0	5000.0	11	0	9	0	0	0	0
258. ph#C3H4Y	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
259. ph#C3H4-1	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
260. ph#C3H4-2	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
261. ph#C3H4-3	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
262. ph#C3H4-4	G	0	117.17208	300.0	5000.0	9	0	9	0	0	0	0
263. indenyl	G	0	115.15614	300.0	5000.0	7	0	9	0	0	0	0
264. naphthyl	G	0	127.16729	200.0	6000.0	7	0	10	0	0	0	0
265. C9H11#-1	G	0	119.18802	300.0	5000.0	11	0	9	0	0	0	0
266. C10H11	G	0	131.19917	300.0	5000.0	11	0	10	0	0	0	0
267. C10H11-1	G	0	131.19917	300.0	5000.0	11	0	10	0	0	0	0
268. C10H11-2	G	0	131.19917	300.0	5000.0	11	0	10	0	0	0	0
269. C10H11-3	G	0	131.19917	300.0	5000.0	11	0	10	0	0	0	0
270. C8H7O#	G	0	119.14439	300.0	5000.0	7	1	8	0	0	0	0
271. C8H7O#-1	G	0	119.14439	300.0	5000.0	7	1	8	0	0	0	0
272. ph#C4H8X	G	0	133.21511	300.0	5000.0	13	0	10	0	0	0	0
273. C3H5C6H4CH2	G	0	131.19917	300.0	5000.0	11	0	10	0	0	0	0

REACTIONS CONSIDERED	A	b	E
1. toluene=benzyl+R1H	2.09E+15	0.0	87510.0
2. toluene=C6H5#+R4CH3	2.66E+16	0.0	97880.0
3. toluene+O2=benzyl+R3OOH	2.18E+07	2.5	46045.0
4. toluene+R1H=C6H6#+R4CH3	5.67E+08	1.4	5650.0
5. toluene+B1O=OC6H4CH3+R1H	1.70E+13	0.0	3600.0
6. toluene+R2OH=HOC6H4CH3+R1H	1.30E+13	0.0	10600.0
7. toluene+R2OH=C6H5OH#+R4CH3	7.83E+02	2.9	3219.3
8. toluene+R1H=benzyl+H2	2.92E+06	2.4	5810.0
9. toluene+B1O=benzyl+R2OH	6.30E+11	0.0	0.0
10. toluene+R2OH=benzyl+H2O	5.20E+09	1.0	870.0
11. toluene+R3OOH=benzyl+H2O2	4.00E+11	0.0	14000.0
12. toluene+R4CH3=benzyl+CH4	3.91E+00	3.8	6980.0
13. toluene+R10C2H3V=benzyl+C2H4Z	4.00E+12	0.0	8000.0
14. toluene+C3H3=benzyl+pC3H4	1.60E+12	0.0	15100.0
15. toluene+C3H5Y=benzyl+C3H6Y	1.60E+12	0.0	15100.0
16. toluene+nC4H5=benzyl+C4H6Z2	1.60E+12	0.0	11100.0
17. toluene+iC4H5=benzyl+C4H6Z2	1.60E+12	0.0	15100.0
18. toluene+C5H5#=benzyl+C5H6#	1.60E+11	0.0	15100.0
19. toluene+R5CHO=benzyl+HCHO	3.77E+13	0.0	23787.4
20. toluene+C6H5#=benzyl+C6H6#	7.94E+13	0.0	11940.0
21. toluene+C6H5O#=benzyl+C6H5OH#	1.60E+12	0.0	15100.0
22. toluene+C6H4CH3=benzyl+toluene	7.90E+13	0.0	12000.0
23. toluene+OC6H4CH3=benzyl+HOC6H4CH3	1.60E+11	0.0	15100.0
24. toluene+C6H5CH2O=benzyl+C6H5CH2OH	1.60E+11	0.0	11100.0
25. toluene+HOC6H4CH2=benzyl+HOC6H4CH3	1.60E+11	0.0	15100.0
26. toluene+R1H=C6H4CH3+H2	1.22E+08	2.0	15880.0
27. toluene+B1O=C6H4CH3+R2OH	2.00E+13	0.0	14700.0
28. toluene+R2OH=C6H4CH3+H2O	1.36E+04	2.7	619.6
29. toluene+R3OOH=C6H4CH3+H2O2	9.20E+12	0.0	28810.0
30. toluene+R4CH3=C6H4CH3+CH4	2.07E+00	3.9	13300.0
31. benzyl=>C5H5#+C2H2	6.00E+13	0.0	70000.0
32. benzyl=>C3H3+C4H4	2.00E+14	0.0	83600.0
33. benzyl=C5H5CCH+R1H	3.16E+15	0.0	85205.0
34. benzyl+O2=C6H5CH2O+B1O	6.30E+12	0.0	40000.0
35. benzyl+B1O=C6H5#+HCHO	3.50E+13	0.0	0.0
36. benzyl+B1O=C6H5CHO+R1H	1.00E+14	0.0	0.0
37. benzyl+R2OH=C6H5CH2OH	5.00E+13	0.0	0.0
38. 2benzyl=bibenzyl	5.01E+12	0.0	454.0
39. benzyl+R4CH3=styrene+H2	4.68E+24	-3.2	27018.0
40. benzyl+R4CH3=>etC6H5	3.00E+13	0.0	0.0

41. etC6H5=>benzyl+R4CH3	2.00E+15	0.0	72700.0
42. C6H4CH3+O2=OC6H4CH3+B1O	2.60E+13	0.0	6100.0
43. C6H4CH3+O2=OC6H4O+R4CH3	3.00E+13	0.0	9000.0
44. C6H4CH3+R1H=toluene	1.00E+14	0.0	0.0
45. C6H4CH3+B1O=OC6H4CH3	1.00E+14	0.0	0.0
46. C6H4CH3+R2OH=HOC6H4CH3	1.00E+13	0.0	0.0
47. C6H4CH3+R4CH3=C8H10#	1.20E+06	2.0	-3700.0
48. C6H4CH3+R3OOH=OC6H4CH3+R2OH	1.50E+13	0.0	0.0
49. C6H4CH3+R1H=benzyl+R1H	1.00E+13	0.0	0.0
50. C6H5CH2O=R1H+C6H5CHO	2.00E+13	0.0	27500.0
51. C6H5CH2O=C6H5#+HCHO	2.00E+13	0.0	27500.0
52. C6H5CH2O+O2=R3OOH+C6H5CHO	6.00E+10	0.0	1600.0
53. OC6H4CH3=>R1H+C6H6#+B2CO	3.00E+11	0.0	43800.0
54. OC6H4CH3=>C2H2+iC4H5+B2CO	3.00E+11	0.0	43800.0
55. OC6H4CH3=>C3H3+aC3H4+B2CO	1.50E+11	0.0	43800.0
56. OC6H4CH3+R1H=HOC6H4CH3	1.00E+14	0.0	0.0
57. C6H5CHO+O2=C6H5CO+R3OOH	7.00E+11	0.0	39500.0
58. C6H5CHO=C6H5CO+R1H	3.98E+15	0.0	83740.0
59. C6H5CHO+R1H=C6H6#+R5CHO	5.80E+13	0.0	8100.0
60. C6H5CHO+R4CH3=toluene+R5CHO	1.20E+12	0.0	15900.0
61. C6H5CHO+R1H=C6H5CO+H2	4.00E+13	0.0	3200.0
62. C6H5CHO+B1O=C6H5CO+R2OH	6.00E+12	0.0	1800.0
63. C6H5CHO+R2OH=C6H5CO+H2O	7.80E+12	0.0	0.0
64. C6H5CHO+R3OOH=C6H5CO+H2O2	3.00E+12	0.0	11000.0
65. C6H5CHO+R4CH3=C6H5CO+CH4	2.00E-06	5.6	1500.0
66. C6H5CHO+R11C2H5=C6H5CO+C2H6	1.30E+12	0.0	7500.0
67. C6H5CHO+C3H5Y=C6H5CO+C3H6Y	1.30E+12	0.0	11500.0
68. C6H5CHO+iC4H5=C6H5CO+C4H6Z2	1.30E+12	0.0	11500.0
69. C6H5CHO+nC4H5=C6H5CO+C4H6Z2	1.30E+12	0.0	7500.0
70. C6H5CHO+benzyl=toluene+C6H5CO	1.30E+11	0.0	11500.0
71. C6H5CHO+C6H5O#=C6H5CO+C6H5OH#	1.30E+11	0.0	11500.0
72. C6H5CHO+OC6H4CH3=C6H5CO+HOC6H4CH3	1.30E+11	0.0	11500.0
73. C6H5CHO+C5H5#=C6H5CO+C5H6#	1.30E+11	0.0	11500.0
74. C6H5CHO+HOC6H4CH2=C6H5CO+HOC6H4CH3	1.30E+11	0.0	11500.0
75. C6H5CHO+C6H5#=C6H5CO+C6H6#	1.30E+11	0.0	11500.0
76. C6H5CO=C6H5#+B2CO	3.98E+14	0.0	29400.0
77. HOC6H4CH3+O2=OC6H4CH3+R3OOH	1.00E+13	0.0	38900.0
78. HOC6H4CH3+O2=HOC6H4CH2+R3OOH	2.10E+12	0.0	38600.0
79. HOC6H4CH3+R1H=C6H5OH#+R4CH3	1.15E+13	0.0	8500.0
80. HOC6H4CH3+R1H=OC6H4CH3+H2	1.20E+14	0.0	12400.0
81. HOC6H4CH3+B1O=OC6H4CH3+R2OH	1.30E+13	0.0	2900.0
82. HOC6H4CH3+R2OH=OC6H4CH3+H2O	1.40E+08	1.4	-960.0

83. HOC6H4CH3+R3OOH=OC6H4CH3+H2O2	1.00E+12	0.0	10000.0
84. HOC6H4CH3+R4CH3=OC6H4CH3+CH4	1.80E+11	0.0	7700.0
85. HOC6H4CH3+C6H5#=OC6H4CH3+C6H6#	4.90E+12	0.0	4400.0
86. HOC6H4CH3+C5H5#=OC6H4CH3+C5H6#	4.90E+11	0.0	9400.0
87. HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y	4.90E+11	0.0	9400.0
88. HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2	4.90E+11	0.0	9400.0
89. HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH#	4.90E+11	0.0	9400.0
90. HOC6H4CH3+R1H=HOC6H4CH2+H2	1.20E+14	0.0	8400.0
91. HOC6H4CH3+B1O=HOC6H4CH2+R2OH	6.30E+11	0.0	0.0
92. HOC6H4CH3+R2OH=HOC6H4CH2+H2O	5.20E+09	1.0	870.0
93. HOC6H4CH3+R3OOH=HOC6H4CH2+H2O2	4.00E+11	0.0	14000.0
94. HOC6H4CH3+R4CH3=HOC6H4CH2+CH4	1.60E+12	0.0	11100.0
95. HOC6H4CH3+C3H5Y=HOC6H4CH2+C3H6Y	1.60E+12	0.0	15100.0
96. HOC6H4CH3+C3H3=HOC6H4CH2+pC3H4	1.60E+12	0.0	15100.0
97. HOC6H4CH3+iC4H5=HOC6H4CH2+C4H6Z2	1.60E+12	0.0	15100.0
98. HOC6H4CH3+nC4H5=HOC6H4CH2+C4H6Z2	1.60E+12	0.0	11100.0
99. HOC6H4CH3+C5H5#=HOC6H4CH2+C5H6#	1.60E+11	0.0	15100.0
100. HOC6H4CH3+C6H5#=HOC6H4CH2+C6H6#	7.90E+13	0.0	12000.0
101. HOC6H4CH3+C6H5O#=HOC6H4CH2+C6H5OH#	1.60E+11	0.0	15100.0
102. HOC6H4CH3+C6H4CH3=HOC6H4CH2+toluene	7.90E+13	0.0	12000.0
103. HOC6H4CH3+OC6H4CH3=HOC6H4CH2+HOC6H4CH3	1.60E+11	0.0	15100.0
104. HOC6H4CH3+C6H5CH2O=HOC6H4CH2+C6H5CH2OH	1.60E+11	0.0	11100.0
105. HOC6H4CH2+O2=HOC6H4CH2OO	4.60E+11	0.0	-377.0
106. HOC6H4CH2+O2=HOC6H4CH2O+B1O	6.30E+12	0.0	40000.0
107. HOC6H4CH2+R3OOH=HOC6H4CH2O+R2OH	1.50E+13	0.0	0.0
108. HOC6H4CH2+R1H=HOC6H4CH3	1.00E+14	0.0	0.0
109. HOC6H4CH2+R4CH3=C6H5OH#+C2H4Z	1.50E+13	0.0	0.0
110. HOC6H4CH2OO=C6H4OHCHO+R2OH	3.40E+09	1.0	37500.0
111. HOC6H4CH2O=R1H+C6H4OHCHO	2.00E+13	0.0	27500.0
112. HOC6H4CH2O=C6H4OH#+HCHO	2.00E+13	0.0	27500.0
113. HOC6H4CH2O+O2=R3OOH+C6H4OHCHO	6.00E+10	0.0	1600.0
114. C6H4OHCHO+R1H=C6H4OHCO+H2	4.00E+13	0.0	3200.0
115. C6H4OHCHO+B1O=C6H4OHCO+R2OH	6.00E+12	0.0	1800.0
116. C6H4OHCHO+R2OH=C6H4OHCO+H2O	7.80E+12	0.0	0.0
117. C6H4OHCHO+R3OOH=C6H4OHCO+H2O2	3.00E+12	0.0	11000.0
118. C6H4OHCHO+R4CH3=C6H4OHCO+CH4	2.00E-06	5.6	1500.0
119. C6H4OHCO=C6H4OH#+B2CO	2.00E+13	0.0	30500.0
120. C6H5CH2OH+O2=R3OOH+C6H5CHOH	1.40E+12	0.0	34000.0
121. C6H5CH2OH+O2=C6H5CH2O+R3OOH	2.00E+14	0.0	41400.0
122. C6H5CH2OH+R1H=C6H6#+R6CH2OH	5.80E+13	0.0	8100.0
123. C6H5CH2OH+R1H=C6H5CHOH+H2	8.00E+13	0.0	6400.0
124. C6H5CH2OH+B1O=C6H5CHOH+R2OH	4.20E+11	0.0	-2000.0

125. C6H5CH2OH+R2OH=C6H5CHOH+H2O	3.50E+09	1.0	-1130.0
126. C6H5CH2OH+R3OOH=C6H5CHOH+H2O2	2.70E+11	0.0	12000.0
127. C6H5CH2OH+R4CH3=C6H5CHOH+CH4	1.10E+12	0.0	9100.0
128. C6H5CH2OH+C3H5Y=C6H5CHOH+C3H6Y	1.10E+12	0.0	13100.0
129. C6H5CH2OH+iC4H5=C6H5CHOH+C4H6Z2	1.10E+12	0.0	13100.0
130. C6H5CH2OH+nC4H5=C6H5CHOH+C4H6Z2	1.11E+00	0.0	13100.0
131. C6H5CH2OH+C6H5#=C6H5CHOH+C6H6#	5.20E+13	0.0	10000.0
132. C6H5CH2OH+C6H4CH3=C6H5CHOH+toluene	5.20E+13	0.0	10000.0
133. C6H5CH2OH+C6H5O#=C6H5CHOH+C6H5OH#	1.10E+11	0.0	13100.0
134. C6H5CH2OH+benzyl=C6H5CHOH+toluene	1.10E+11	0.0	13100.0
135. C6H5CH2OH+OC6H4CH3=C6H5CHOH+HOC6H4CH3	1.10E+11	0.0	13100.0
136. C6H5CH2OH+HOC6H4CH2=C6H5CHOH+HOC6H4CH3	1.10E+11	0.0	13100.0
137. C6H5CH2OH+C5H5#=C6H5CHOH+C5H6#	1.10E+11	0.0	13100.0
138. C6H5CHOH=C6H5CHO+R1H	2.00E+14	0.0	23300.0
139. etC6H5=R1H+C8H9#	4.30E+14	0.0	83600.0
140. etC6H5+O2=C8H9#+R3OOH	1.40E+12	0.0	34000.0
141. etC6H5+O2=C8H9#-1+R3OOH	1.20E+13	0.0	49000.0
142. etC6H5+R1H=C6H6#+R11C2H5	5.80E+13	0.0	8100.0
143. etC6H5+R4CH3=toluene+R11C2H5	1.20E+12	0.0	15900.0
144. etC6H5+R1H=C8H9#+H2	8.00E+13	0.0	6400.0
145. etC6H5+B1O=C8H9#+R2OH	4.20E+11	0.0	-2.0
146. etC6H5+R2OH=C8H9#+H2O	3.50E+09	1.0	-1130.0
147. etC6H5+R3OOH=C8H9#+H2O2	2.70E+11	0.0	12000.0
148. etC6H5+R4CH3=C8H9#+CH4	1.10E+12	0.0	9100.0
149. etC6H5+C3H5Y=C8H9#+C3H6Y	1.10E+12	0.0	13100.0
150. etC6H5+iC4H5=C8H9#+C4H6Z2	1.10E+12	0.0	13100.0
151. etC6H5+nC4H5=C8H9#+C4H6Z2	1.11E+00	0.0	13100.0
152. etC6H5+C6H5O#=C8H9#+C6H5OH#	1.10E+11	0.0	13100.0
153. etC6H5+benzyl=C8H9#+toluene	1.10E+11	0.0	13100.0
154. etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3	1.10E+11	0.0	13100.0
155. etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3	1.10E+11	0.0	13100.0
156. etC6H5+C5H5#=C8H9#+C5H6#	1.10E+11	0.0	13100.0
157. etC6H5+R1H=C8H9#-1+H2	2.80E+07	2.0	7700.0
158. etC6H5+B1O=C8H9#-1+R2OH	5.10E+13	0.0	7850.0
159. etC6H5+R2OH=C8H9#-1+H2O	2.70E+06	2.0	450.0
160. etC6H5+R3OOH=C8H9#-1+H2O2	6.00E+11	0.0	17000.0
161. etC6H5+R4CH3=C8H9#-1+CH4	3.00E-01	4.0	8200.0
162. C8H9#-1=C2H4Z+C6H5#	7.10E+14	0.0	43500.0
163. C8H9#=R1H+styrene	3.10E+13	0.0	50670.0
164. C8H9#-1=R1H+styrene	1.60E+13	0.0	34800.0
165. C8H9#+O2=R3OOH+styrene	7.00E+11	0.0	15000.0
166. C8H9#+R3OOH=R2OH+R4CH3+C6H5CHO	1.50E+13	0.0	0.0

167. C8H9#-1+O2=R3OOH+styrene	1.50E+12	0.0	5000.0
168. C8H9#-1+R3OOH=R2OH+HCHO+benzyl	1.50E+13	0.0	0.0
169. styrene+O2=R3OOH+C6H5C2H2	2.00E+13	0.0	57900.0
170. styrene+B1O=benzyl+R1H+B2CO	3.00E+08	1.4	900.0
171. styrene+R2OH=benzyl+HCHO	1.40E+12	0.0	-900.0
172. styrene+R2OH=C6H5CHO+R4CH3	2.80E+12	0.0	-900.0
173. styrene+R1H=C6H5C2H2+H2	6.60E+05	2.5	9200.0
174. styrene+R2OH=C6H5C2H2+H2O	1.50E+06	2.0	400.0
175. styrene+R4CH3=C6H5C2H2+CH4	3.50E+13	0.0	15500.0
176. styrene+R4CH3=toluene+R10C2H3V	1.20E+12	0.0	15900.0
177. C6H5C2H2+O2=C6H5CO+HCHO	4.50E+16	-1.4	1000.0
178. C6H5C2H2+R1H=C6H5#C2H+H2	1.00E+13	0.0	0.0
179. C6H5C2H2+R2OH=C6H5#C2H+H2O	1.00E+13	0.0	0.0
180. C6H5C2H2+R4CH3=ph#C3H5Z	1.50E+13	0.0	0.0
181. C6H5C2H2+R4CH3=ph#C3H5p	1.50E+13	0.0	0.0
182. C5H5CCH=C5H5#+R9C2H	4.20E+15	0.0	125000.0
183. C5H5CCH+R1H=C5H5#+C2H2	2.00E+10	0.0	0.0
184. C5H5CCH+R1H=C3H3+C4H4	6.00E+10	0.0	0.0
185. C5H5CCH+R2OH=C5H5#+CH2COZ	4.30E+11	0.0	-800.0
186. C5H4CCH2=C5H5CCH	2.50E+12	0.0	59000.0
187. C5H4CCH2+R1H=C5H5CCH+R1H	8.50E+12	0.0	2000.0
188. C5H4CCH2+R2OH=C5H5#+CH2COZ	2.00E+12	0.0	-200.0
189. bibenzyl=C14H13#+R1H	1.00E+16	0.0	83660.0
190. bibenzyl+O2=C14H13#+R3OOH	2.80E+12	0.0	35000.0
191. bibenzyl+R1H=C14H13#+H2	5.40E+04	2.5	-1900.0
192. bibenzyl+B1O=C14H13#+R2OH	8.40E+11	0.0	-2.0
193. bibenzyl+R2OH=C14H13#+H2O	7.00E+09	1.0	-1130.0
194. bibenzyl+R3OOH=C14H13#+H2O2	5.40E+11	0.0	12000.0
195. bibenzyl+R4CH3=C14H13#+CH4	2.20E+12	0.0	9100.0
196. bibenzyl+C6H5O#=C14H13#+C6H5OH#	2.20E+12	0.0	13100.0
197. bibenzyl+benzyl=C14H13#+toluene	2.20E+12	0.0	9100.0
198. bibenzyl+C3H5Y=C14H13#+C3H6Y	2.20E+12	0.0	13100.0
199. C14H13#=stilbene+R1H	7.94E+15	0.0	51864.0
200. C6H5C2H2=C6H5#C2H+R1H	4.00E+12	0.0	47500.0
201. C6H5C2H2+R1H=styrene	2.00E+13	0.0	0.0
202. C6H5#C2H+B1O=>C6H5#+R12CHCOZ	9.04E+12	0.0	4530.0
203. C6H5#C2H+R2OH=C6H5#+CH2COZ	7.50E+06	1.6	2106.0
204. C6H5#C2H+O2=C6H5CO+R5CHO	2.20E+07	1.5	33100.0
205. C6H5#C2H+R4CH3=>toluene+R9C2H	1.20E+12	0.0	15900.0
206. toluene+R4CH3=>C8H10#+R1H	1.99E+12	0.0	15940.0
207. C8H9#+R4CH3=cumene	1.50E+13	0.0	0.0
208. C6H5#+iC3H7=cumene	1.50E+13	0.0	0.0

209. cumene+O2=>CH3styre+R1H+R3OOH	1.40E+12	0.0	33620.0
210. cumene+O2=C9H11#-1+R3OOH	2.40E+13	0.0	52300.0
211. B1O+cumene=>R2OH+CH3styre+R1H	3.40E+10	0.0	1330.0
212. B1O+cumene=R2OH+C9H11#-1	1.02E+14	0.0	7850.0
213. cumene+R1H=>H2+CH3styre+R1H	2.50E+04	2.5	-2790.0
214. cumene+R1H=H2+C9H11#-1	5.70E+07	2.0	7700.0
215. cumene+R2OH=>H2O+CH3styre+R1H	1.30E+06	2.0	-2620.0
216. cumene+R2OH=H2O+C9H11#-1	5.34E+06	2.0	450.0
217. cumene+R3OOH=>H2O2+CH3styre+R1H	1.60E+04	2.6	10900.0
218. cumene+R3OOH=H2O2+C9H11#-1	1.20E+12	0.0	17000.0
219. cumene+R4CH3=>CH4+CH3styre+R1H	5.00E+10	0.0	5600.0
220. cumene+R4CH3=CH4+C9H11#-1	6.00E-01	4.0	8200.0
221. C9H11#-1=styrene+R4CH3	2.00E+13	0.0	31000.0
222. C9H11#-1=C3H6Y+C6H5#	2.00E+13	0.0	38500.0
223. C9H11#-1=CH3styre+R1H	1.60E+13	0.0	34300.0
224. C9H11#-1+R1H=cumene	1.00E+14	0.0	0.0
225. CH3styre+R1H=C2H3C6H4CH2+H2	1.70E+05	2.5	2500.0
226. CH3styre+R2OH=C2H3C6H4CH2+H2O	3.00E+06	2.0	-298.0
227. C6H5C2H2+R4CH3=CH3styre	1.50E+13	0.0	0.0
228. CH3styre+R1H=styrene+R4CH3	5.80E+13	0.0	8100.0
229. CH3styre+R1H=toluene+R10C2H3V	5.80E+13	0.0	8100.0
230. CH3styre+O2=>aC3H4+C6H5#+R3OOH	1.20E+13	0.0	49000.0
231. B1O+CH3styre=>R2OH+aC3H4+C6H5#	5.10E+13	0.0	7850.0
232. CH3styre+R1H=>H2+aC3H4+C6H5#	2.85E+07	2.0	7700.0
233. CH3styre+R2OH=>H2O+aC3H4+C6H5#	2.67E+06	2.0	450.0
234. CH3styre+R3OOH=>H2O2+aC3H4+C6H5#	6.00E+11	0.0	17000.0
235. CH3styre+R4CH3=>CH4+aC3H4+C6H5#	3.00E-01	4.0	8200.0
236. indane=>CH3styre	1.26E+16	0.0	84900.0
237. R1H+indanyl-Y=indane	1.00E+14	0.0	0.0
238. R1H+indanyl-1=indane	1.00E+14	0.0	0.0
239. indane+O2=indanyl-Y+R3OOH	2.80E+12	0.0	35960.0
240. indane+O2=indanyl-1+R3OOH	1.40E+13	0.0	45460.0
241. indane+R1H=ph#C3H6-1	2.32E+14	0.0	8100.0
242. indane+R4CH3=CH3C6H4C3H6	2.40E+12	0.0	15900.0
243. indane+B1O=>C6H5O#+C3H5Y	1.70E+13	-0.1	3600.0
244. indane+R1H=indanyl-Y+H2	1.08E+05	2.5	-1900.0
245. indane+R1H=indanyl-1+H2	9.00E+06	2.0	5000.0
246. indane+B1O=indanyl-Y+R2OH	1.70E+11	0.7	3250.0
247. indane+B1O=indanyl-1+R2OH	2.60E+13	0.0	5200.0
248. indane+R2OH=indanyl-Y+H2O	6.00E+06	2.0	-1520.0
249. indane+R2OH=indanyl-1+H2O	2.60E+06	2.0	-770.0
250. indane+R3OOH=indanyl-Y+H2O2	1.28E+04	2.6	12400.0

251. indane+R3OOH=indanyl-1+H2O2	4.00E+11	0.0	15500.0
252. indane+R4CH3=indanyl-Y+CH4	2.00E+11	0.0	7300.0
253. indane+R4CH3=indanyl-1+CH4	2.00E+11	0.0	9600.0
254. indane+C6H5#=indanyl-Y+C6H6#	8.00E+12	0.0	8000.0
255. indane+benzyl=indanyl-Y+toluene	8.80E+12	0.0	13100.0
256. indanyl-Y=C2H3C6H4CH2	1.36E+12	0.4	41330.0
257. indanyl-Y=indene+R1H	1.21E+11	1.0	42200.0
258. indanyl-Y+R3OOH=>C9H9O#+R2OH	1.00E+13	0.0	0.0
259. indanyl-Y+B1O=C9H9O#	1.16E+14	0.0	20.0
260. indanyl-Y+R4CH3=methylindane	1.00E+13	0.0	0.0
261. indanyl-Y+benzyl=toluene+indene	1.00E+13	0.0	0.0
262. indanyl-Y+R1H=indene+H2	1.80E+13	0.0	0.0
263. indanyl-Y+R2OH=indene+H2O	6.00E+12	0.0	0.0
264. indanyl-Y+indanyl-Y=indene+indane	5.00E+12	0.0	0.0
265. indanyl-Y+indenyl=2indene	5.00E+12	0.0	0.0
266. indanyl-Y+O2=indene+R3OOH	1.58E+12	0.0	15200.0
267. indanyl-1=indanyl-Y	1.95E+10	1.0	34200.0
268. C9H9O#=C9H8O#+R1H	9.77E+12	0.0	17300.0
269. C9H9O#=>C6H6#+B2CO+R10C2H3V	2.80E+13	0.0	17100.0
270. C9H9O#=styrene+R5CHO	2.80E+13	0.0	17100.0
271. C2H3C6H4CH2+R1H=CH3styre	1.00E+14	0.0	0.0
272. C2H3C6H4CH2+O2=C2H3C6H4CH2O+B1O	6.30E+12	0.0	40000.0
273. C2H3C6H4CH2+B1O=C6H5C2H2+HCHO	3.50E+13	0.0	0.0
274. C2H3C6H4CH2+B1O=C2H3C6H4CHO+R1H	1.00E+14	0.0	0.0
275. C2H3C6H4CH2+R3OOH=C2H3C6H4CH2O+R2OH	5.00E+12	0.0	0.0
276. C2H3C6H4CH2O=R1H+C2H3C6H4CHO	2.00E+13	0.0	27500.0
277. C2H3C6H4CH2O=C6H5C2H2+HCHO	2.00E+13	0.0	27500.0
278. C2H3C6H4CH2O+O2=R3OOH+C2H3C6H4CHO	6.00E+10	0.0	1600.0
279. indanyl-1=indene+R1H	6.57E+10	0.9	35770.0
280. indanyl-1=C3H5C6H4	1.11E+13	0.1	45870.0
281. indanyl-1+O2=indene+R3OOH	3.16E+12	0.0	5000.0
282. ph#C3H6-1=benzyl+C2H4Z	3.30E+13	0.0	22500.0
283. ph#C3H6-1=ph#C3H5Z+R1H	3.00E+13	0.0	38000.0
284. ph#C3H6-2=C6H5#+C3H6Y	2.00E+13	0.0	34500.0
285. ph#C3H6-2=ph#C3H5p+R1H	3.20E+13	0.0	34800.0
286. ph#C3H6-2=ph#C3H5Z+R1H	3.00E+13	0.0	38000.0
287. ph#C3H6-Y=R1H+ph#C3H5p	3.00E+13	0.0	50500.0
288. ph#C3H6-Y=styrene+R4CH3	1.30E+13	0.0	35900.0
289. ph#C3H6-2=ph#C3H6-Y	1.95E+10	1.0	34200.0
290. ph#C3H6-2=ph#C3H6-1	1.95E+10	1.0	38700.0
291. ph#C3H6-1=ph#C3H6-Y	3.40E+09	1.0	32500.0
292. ph#C3H6-1+O2=ph#C3H5Z+R3OOH	1.58E+12	0.0	5000.0

293. ph#C3H6-2+O2=ph#C3H5p+R3OOH	2.60E+11	0.0	2500.0
294. ph#C3H6-2+O2=ph#C3H5Z+R3OOH	1.58E+12	0.0	5000.0
295. ph#C3H6-Y+O2=ph#C3H5p+R3OOH	1.58E+12	0.0	15200.
296. ph#C3H6-Y+R1H=ph#C3H7	1.00E+14	0.0	0.0
297. CH3C6H4C3H6=o-methylbenzyl+C2H4Z	3.30E+13	0.0	22500.0
298. C3H5C6H4+O2=C3H5C6H4O+B1O	2.60E+13	0.0	6100.0
299. C3H5C6H4=ph#C3H4Y	3.40E+13	0.0	34500.0
300. C3H5C6H4O=>C6H6#+B2CO+R10C2H3V	3.00E+11	0.0	43800.0
301. C3H5C6H4O=>C2H2+B2CO+C4H4+R10C2H3V	3.00E+11	0.0	43800.0
302. C3H5C6H4O=>C3H3+lC5H6+B2CO	1.50E+11	0.0	43800.0
303. ph#C3H4-1=ph#C3H4Y	3.40E+13	0.0	34500.0
304. ph#C3H4-2=ph#C3H4Y	1.30E+13	0.0	44500.0
305. ph#C3H4-3=ph#C3H4Y	5.00E+13	0.0	37000.0
306. ph#C3H4-4=ph#C3H4Y	2.00E+13	0.0	47000.0
307. ph#C3H4-1=benzyl+C2H2	2.00E+13	0.0	30000.0
308. ph#C3H4-2=C6H5#+aC3H4	2.00E+13	0.0	35500.0
309. ph#C3H4-3=C6H5#C2H+R4CH3	2.00E+13	0.0	31500.0
310. ph#C3H4-4=C6H5#+pC3H4	2.00E+13	0.0	31000.0
311. ph#C3H4Y+R1H=ph#C3H5Z	5.00E+13	0.0	0.0
312. ph#C3H4Y+R1H=ph#C3H5p	5.00E+13	0.0	0.0
313. ph#C3H4Y+R4CH3=ph#C4H7-3	5.00E+12	0.0	0.0
314. ph#C3H4Y+R3OOH=R2OH+R10C2H3V+C6H5CHO	5.00E+12	0.0	0.0
315. ph#C3H4Y=>C5H5#+C4H4	6.00E+13	0.0	70000.0
316. ph#C3H4Y+B1O=C6H5#+C2H3CHO	3.50E+13	0.0	0.0
317. ph#C3H4Y+B1O=C6H5CHO+R10C2H3V	1.00E+14	0.0	0.0
318. indene+R2OH=>C2H4Z+C6H5CO	1.37E+12	0.0	-1040.0
319. indene+R2OH=>R10C2H3V+B2CO+C6H6#	1.37E+12	0.0	-1040.0
320. indene+R2OH=>o-methylbenzyl+B2CO	1.37E+12	0.0	-1040.0
321. indene+O2=R3OOH+indenyl	1.40E+12	0.0	28080.0
322. indene+B1O=indenyl+R2OH	1.76E+11	0.7	3250.0
323. indene+R1H=indenyl+H2	1.08E+05	2.5	-1900.0
324. indene+R2OH=indenyl+H2O	6.00E+06	2.0	-1520.0
325. indene+R4CH3=indenyl+CH4	2.00E+11	0.0	7300.0
326. indene+R3OOH=H2O2+indenyl	1.28E+04	2.6	12400.0
327. indene+R1H=ph#C3H4Y	5.80E+13	0.0	8100.0
328. indene+R1H=ph#C3H4-1	5.80E+13	0.0	8100.0
329. indenyl=C5H5#+C4H2	5.00E+13	0.0	75000.0
330. indenyl+R1H=indene	1.00E+14	0.0	0.0
331. C6H5#+C3H3=indene	6.46E+12	0.0	0.0
332. indenyl+R4CH3=methylindene	1.50E+13	0.0	0.0
333. indenyl+R3OOH=C9H7O#+R2OH	3.00E+12	0.0	0.0
334. indenyl+B1O=C9H7O#	5.80E+13	0.0	20.0

335. indenyl+R2OH=>styrene+B2CO	4.00E+14	0.0	4500.0
336. C9H7O#=C9H6O#+R1H	2.00E+13	0.0	27500.0
337. C9H7O#=>C6H6#+B2CO+R9C2H	2.80E+13	0.0	17100.0
338. C9H7O#=C6H5#C2H+R5CHO	2.80E+13	0.0	17100.0
339. methylindane+R1H=>benzyl+C3H6Y	5.80E+13	0.0	8100.0
340. methylindane+R1H=>C2H4Z+C8H9#	5.80E+13	0.0	8100.0
341. methylindane+R1H=C10H11+H2	5.00E+04	2.5	-1900.0
342. methylindane+R1H=C10H11-1+H2	9.00E+06	2.0	5000.0
343. methylindane+R1H=C10H11-2+H2	2.90E+07	2.0	7700.0
344. methylindane+R1H=C10H11-3+H2	2.50E+04	2.5	-2790.0
345. methylindane+R2OH=C10H11+H2O	3.00E+06	2.0	-1520.0
346. methylindane+R2OH=C10H11-1+H2O	2.60E+06	2.0	-770.0
347. methylindane+R2OH=C10H11-2+H2O	2.70E+06	2.0	450.0
348. methylindane+R2OH=C10H11-3+H2O	1.30E+06	2.0	-2620.0
349. C10H11-1=C10H11	1.95E+10	1.0	34200.0
350. C10H11=methylindene+R1H	1.21E+11	1.0	42200.0
351. C10H11-1=R4CH3+indene	2.00E+13	0.0	31000.0
352. C10H11+O2=R3OOH+methylindene	1.58E+12	0.0	15200.0
353. C10H11-1+O2=R3OOH+methylindene	2.60E+11	0.0	2500.0
354. C10H11-1+O2=R3OOH+methylindene-2	2.60E+11	0.0	2500.0
355. C10H11-3+O2=R3OOH+methylindene-2	1.58E+12	0.0	15200.0
356. C10H11+R1H=methylindane	1.00E+14	0.0	0.0
357. C10H11-2=C6H5C2H2+C2H4Z	2.00E+13	0.0	28700.0
358. C10H11-3+R1H=methylindane	1.00E+14	0.0	0.0
359. C10H11-3=methylindene-2+R1H	1.21E+11	1.0	42200.0
360. C10H11-3=C3H5C6H4CH2	1.36E+12	0.4	41330.0
361. C3H5C6H4CH2+R1H=C3H5C6H4CH3	1.00E+14	0.0	0.0
362. methylindene+B1O=C6H5C2H2+C2H2+R2OH	5.10E+13	0.0	7850.0
363. methylindene+B1O=naphthalene+R1H+R2OH	5.10E+13	0.0	7850.0
364. methylindene-2+B1O=naphthalene+R1H+R2OH	5.10E+13	0.0	7850.0
365. methylindene+R1H=C6H5C2H2+C2H2+H2	2.85E+07	2.0	7700.0
366. methylindene+R1H=naphthalene+R1H+H2	2.85E+07	2.0	7700.0
367. methylindene-2+R1H=naphthalene+R1H+H2	2.85E+07	2.0	7700.0
368. methylindene+R2OH=C6H5C2H2+C2H2+H2O	2.67E+06	2.0	450.0
369. methylindene+R2OH=naphthalene+R1H+H2O	2.67E+06	2.0	450.0
370. methylindene-2+R2OH=naphthalene+R1H+H2O	2.67E+06	2.0	450.0
371. methylindene+R4CH3=C6H5C2H2+C2H2+CH4	3.00E-01	4.0	8200.0
372. methylindene+R4CH3=naphthalene+R1H+CH4	3.00E-01	4.0	8200.0
373. methylindene-2+R4CH3=naphthalene+R1H+CH4	3.00E-01	4.0	8200.0
374. methylindene+R1H=C10H11-1	2.60E+13	0.0	3200.0
375. methylindene+R1H=>C2H2+C8H9#	5.80E+13	0.0	8100.0
376. C9H8O#+R1H=styrene+R1H+B2CO	5.80E+13	0.0	8100.0

377. C9H8O#+B1O=styrene+CO2	1.00E+13	0.0	2000.0
378. C9H6O#+R1H=C6H5#C2H+R1H+B2CO	5.80E+13	0.0	8100.0
379. C9H6O#+B1O=C6H5#C2H+CO2	1.00E+13	0.0	2000.0
380. 2C5H5#=naphthalene+H2	4.30E+36	-6.3	22835.0
381. C6H5#+iC4H3=naphthalene	3.18E+23	-3.2	2130.0
382. C6H5#+C4H4=naphthalene+R1H	3.30E+33	-5.7	12750.0
383. benzyl+C3H3=naphthalene+R1H+R1H	6.00E+11	0.0	0.0
384. C6H5C2H2+C2H2=naphthalene+R1H	1.60E+16	-1.3	3300.0
385. naphthalene+O2=R3OOH+naphthyl	8.00E+13	0.0	63400.0
386. naphthalene+B1O=>indenyl+B2CO+R1H	2.70E+13	0.0	3600.0
387. naphthalene+R1H=naphthyl+H2	8.00E+08	1.8	16800.0
388. naphthalene+B1O=naphthyl+R2OH	2.70E+13	0.0	14700.0
389. naphthalene+R2OH=naphthyl+H2O	2.10E+08	1.4	1450.0
390. naphthalene+R3OOH=naphthyl+H2O2	7.30E+12	0.0	28900.0
391. naphthalene+R4CH3=naphthyl+CH4	2.70E+12	0.0	15000.0
392. naphthalene+R9C2H=A2C2H+R1H	5.00E+13	0.0	0.0
393. naphthalene+B5CH2=A2CH3	2.20E+13	0.0	4370.0
394. naphthalene+B6CH2=A2CH3	4.40E+13	0.0	4370.0
395. naphthyl+R1H=naphthalene	1.00E+14	0.0	0.0
396. naphthyl+O2=>indenyl+B2CO+B1O	2.60E+13	0.0	6100.0
397. naphthyl+B1O=>indenyl+B2CO	1.00E+14	0.0	0.0
398. naphthyl+R3OOH=>indenyl+B2CO+R2OH	5.00E+12	0.0	0.0
399. naphthyl+R2OH=>indenyl+B2CO+R1H	1.00E+13	0.0	0.0
400. naphthyl+C2H2=A2C2H+R1H	1.30E+24	-3.1	11300.0
401. naphthyl+C2H2=A2R5+R1H	1.90E+31	-5.3	10500.0
402. A2C2H+R1H=A2R5+R1H	4.60E+37	-7.0	11550.0
403. A2R5=C6H5#C2H+C4H2	1.00E+10	0.0	40000.0
404. A2C2H+R2OH=naphthyl+CH2COZ	2.18E-04	4.5	-500.0
405. indenyl+C3H3=A2C2H+2R1H	6.00E+11	0.0	0.0
406. A2CH3=naphthyl+R4CH3	1.00E+16	0.0	48800.0
407. A2CH3=A2CH2+R1H	2.81E+15	0.0	44700.0
408. A2CH3+O2=A2CH2+R3OOH	3.00E+14	0.0	20808.0
409. A2CH3+B1O=A2CH2+R2OH	1.20E+13	0.0	647.0
410. A2CH3+R1H=A2CH2+H2	3.98E+02	3.4	1560.0
411. A2CH3+R1H=naphthalene+R4CH3	1.20E+13	0.0	2550.0
412. A2CH3+R2OH=A2CH2+H2O	5.19E+08	1.0	440.0
413. A2CH3+R3OOH=A2CH2+H2O2	4.00E+11	0.0	7000.0
414. A2CH3+R4CH3=A2CH2+CH4	1.58E+12	0.0	5500.0
415. A2CH2+B1O=naphthyl+HCHO	1.65E+14	0.0	0.0
416. A2CH2+R3OOH=naphthyl+HCHO+R2OH	1.00E+13	0.0	0.0
417. A2CH2+B5CH2=A2C2H+H2+R1H	2.40E+14	0.0	0.0
418. A2CH2+C3H3=phenanthrene+2R1H	5.00E+12	0.0	0.0

419. indenyl+C5H5#=phenanthrene+2R1H	4.30E+12	0.0	4890.0
420. phenanthrene=naphthalene+C4H2	1.00E+10	0.0	45000.0
421. phenanthrene=A2R5+C2H2	2.00E+10	0.0	45000.0
422. phenanthrene+B1O=A2C2H+CH2COZ	2.20E+13	0.0	2765.0
423. phenanthrene+R2OH=A2C2H+CH2COZ+R1H	1.30E+13	0.0	5000.0
424. phenanthrene+B5CH2=CH3phenanth	2.20E+13	0.0	3596.0
425. phenanthrene+B6CH2=CH3phenanth	4.20E+13	0.0	3596.0
426. antra=phenanthrene	7.94E+12	0.0	65000.0
427. CH3phenanth=CH2phenanth+R1H	2.81E+15	0.0	44700.0
428. CH3phenanth+O2=CH2phenanth+R3OOH	3.00E+14	0.0	20808.0
429. CH3phenanth+B1O=CH2phenanth+R2OH	1.20E+13	0.0	642.5
430. CH3phenanth+R1H=phenanthrene+R4CH3	1.20E+13	0.0	2550.0
431. CH3phenanth+R1H=CH2phenanth+H2	1.20E+14	0.0	4200.0
432. CH3phenanth+R2OH=CH2phenanth+H2O	1.26E+13	0.0	1275.0
433. CH3phenanth+R3OOH=CH2phenanth+H2O2	4.00E+11	0.0	7000.0
434. CH3phenanth+R4CH3=CH2phenanth+CH4	1.58E+12	0.0	5500.0
435. CH2phenanth+B5CH2=pyrene+H2+R1H	2.40E+14	0.0	0.0
436. pyrene=C4H2+A2R5	1.00E+10	0.0	45000.0
437. naphthyl+C6H6#=pyrene+R1H+H2	1.00E+12	0.0	2500.0
438. naphthyl+C6H5#=>pyrene+H2	4.30E+37	-6.3	22530.0
439. chrysene=C4H2+phenanthrene	1.00E+10	0.0	45000.0
440. chrysene=C2H2+pyrene	1.00E+10	0.0	45000.0
441. naphthyl+R2OH=naphtol	1.00E+13	0.0	0.0
442. naphtol+R1H=A2O+H2	1.20E+14	0.0	12400.0
443. naphtol+B1O=A2O+R2OH	1.30E+13	0.0	2900.0
444. naphtol+R2OH=A2O+H2O	1.40E+08	1.4	-960.0
445. naphtol+R3OOH=A2O+H2O2	1.00E+12	0.0	10000.0
446. naphtol+R4CH3=A2O+CH4	1.80E+11	0.0	7700.0
447. A2O+R1H=naphtol	1.00E+14	0.0	0.0
448. C3H5C6H4CH3+R1H=toluene+C3H5Y	5.80E+13	0.0	8100.0
449. C3H5C6H4CH3+R1H=ph#C3H5Z+R4CH3	5.80E+13	0.0	8100.0
450. ph#C3H5Z+B1O=>benzyl+R13CH2CHO	6.40E+04	2.6	-1130.0
451. ph#C3H5Z+R2OH=>HCHO+C8H9#-1	1.37E+12	0.0	-1040.0
452. ph#C3H5Z+R4CH3=>benzyl+C3H6Y	1.69E+11	0.0	7400.0
453. ph#C3H5Z+R4CH3=>toluene+C3H5Y	1.20E+12	0.0	15900.0
454. ph#C3H5Z+R1H=>C6H6#+C3H5Y	5.80E+13	0.0	8100.0
455. ph#C3H5Z+B1O=ph#C3H4Y+R2OH	8.80E+10	0.7	3250.0
456. ph#C3H5Z+R1H=ph#C3H4Y+H2	5.40E+04	2.5	-1900.0
457. ph#C3H5Z+R2OH=ph#C3H4Y+H2O	3.00E+06	2.0	-1520.0
458. ph#C3H5Z+R4CH3=ph#C3H4Y+CH4	1.00E+11	0.0	7300.0
459. ph#C3H5Z+R3OOH=ph#C3H4Y+H2O2	6.40E+03	2.6	12400.0
460. ph#C3H5p+R2OH=>benzyl+CH3CHO	1.37E+12	0.0	-1040.0

461. ph#C3H5p+R2OH=>C6H5CHO+R11C2H5				1.37E+12	0.0	-1040.0
462. ph#C3H5p+R1H=>C6H6#+C3H5Y				5.80E+13	0.0	8100.0
463. ph#C3H5p+R4CH3=>toluene+C3H5Y				1.20E+12	0.0	15900.0
464. ph#C3H5p+R4CH3=>benzyl+C3H6Y				1.69E+11	0.0	7400.0
465. ph#C3H5p+R1H=ph#C3H4Y+H2				5.80E+04	2.5	2510.0
466. ph#C3H5p+B1O=ph#C3H4Y+R2OH				5.80E+10	0.7	5900.0
467. ph#C3H5p+R2OH=H2O+ph#C3H4Y				1.00E+06	2.0	-298.0
468. ph#C3H5p+R4CH3=ph#C3H4Y+CH4				7.40E-01	3.5	5670.0
469. ph#C3H5p+R3OOH=ph#C3H4Y+H2O2				3.20E+03	2.6	13900.0
470. ph#C3H7+R1H=C6H6#+nC3H7				5.80E+13	0.0	8100.0
471. ph#C3H7+R4CH3=toluene+nC3H7				1.20E+12	0.0	15900.0
472. ph#C3H7+R1H=ph#C3H6-Y+H2				5.40E+04	2.5	-1900.0
473. ph#C3H7+B1O=ph#C3H6-Y+R2OH				8.80E+10	0.7	3250.0
474. ph#C3H7+R2OH=ph#C3H6-Y+H2O				3.00E+06	2.0	-1520.0
475. ph#C3H7+R3OOH=ph#C3H6-Y+H2O2				6.40E+03	2.6	12400.0
476. ph#C3H7+R4CH3=ph#C3H6-Y+CH4				1.00E+11	0.0	7300.0
477. ph#C4H9+R1H=C6H6#+R20C4H9				5.80E+13	0.0	8100.0
478. ph#C4H9+R4CH3=toluene+R20C4H9				1.20E+12	0.0	15900.0
479. ph#C4H9+R1H=ph#C4H8X+H2				5.40E+04	2.5	-1900.0
480. ph#C4H9+B1O=ph#C4H8X+R2OH				8.80E+10	0.7	3250.0
481. ph#C4H9+R2OH=ph#C4H8X+H2O				3.00E+06	2.0	-1520.0
482. ph#C4H9+R3OOH=ph#C4H8X+H2O2				6.40E+03	2.6	12400.0
483. ph#C4H9+R4CH3=ph#C4H8X+CH4				1.00E+11	0.0	7300.0
484. ph#C4H8X=styrene+R11C2H5				1.30E+13	0.0	35900.0
485. ph#C4H8X+R1H=ph#C4H9				1.00E+14	0.0	0.0
486. C6H5#+R1H(+M)=C6H6#(+M)				1.00E+14	0.0	0.0
Low pressure limit:	0.66000E+76	-0.16300E+02	0.70000E+04			
TROE centering:	0.10000E+01	0.10000E+00	0.58500E+03	0.61130E+04		
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
AR	Enhanced by	3.500E-01				
C6H6#	Enhanced by	3.000E+00				
487. C6H6#+O2=C6H5#+R3OOH				6.00E+13	0.0	63400.0
488. C6H6#+R1H=C6H7#				3.20E+13	0.0	3200.0
489. C6H6#+B1O=C6H5OH#				1.00E+14	-0.3	4674.0
490. C6H6#+B1O=C5H6#+B2CO				3.20E+13	-0.3	4674.0
491. C6H6#+R2OH=C6H5OH#+R1H				1.30E+13	0.0	10600.0
Declared duplicate reaction...						
492. C6H6#+R2OH=C6H5OH#+R1H				1.43E+04	2.6	1134.0
Declared duplicate reaction...						

493. C6H6#+R9C2H=C6H5#C2H+R1H	5.00E+13	0.0	0.0
494. C6H6#+R10C2H3V=styrene+R1H	7.90E+11	0.0	6400.0
495. C6H6#+R1H=C6H5#+H2	1.22E+08	2.0	15880.0
496. C6H6#+B1O=C6H5#+R2OH	2.00E+13	0.0	14700.0
497. C6H6#+R2OH=C6H5#+H2O	1.36E+04	2.7	619.6
498. C6H6#+R3OOH=C6H5#+H2O2	9.20E+12	0.0	28810.0
499. C6H6#+R4CH3=C6H5#+CH4	2.07E+00	3.9	13300.0
500. C6H6#+R11C2H5=C6H5#+C2H6	6.30E+11	0.0	15000.0
501. C6H6#+C3H5Y=C6H5#+C3H6Y	6.30E+11	0.0	20000.0
502. C6H6#+nC4H5=C6H5#+C4H6Z2	6.30E+11	0.0	15000.0
503. C6H6#+iC4H5=C6H5#+C4H6Z2	6.30E+11	0.0	20000.0
504. fulvene+R1H=C6H6#+R1H	3.00E+12	0.5	2000.0
505. fulvene=C6H6#	5.62E+81	-19.4	121500.0
506. fulvene=C6H5#+R1H	2.57E+97	-23.2	153470.0
507. C3H3+C3H3=fulvene	1.26E+56	-12.6	23520.0
508. C3H3+C3H5Y=>fulvene+2R1H	3.26E+29	-5.4	3390.0
509. C6H7#=lC6H7	2.50E+14	0.7	41800.0
510. C6H7#+O2=C6H6#+R3OOH	7.90E+11	0.0	9900.0
511. C6H7#+R1H=C6H8#	1.00E+14	0.0	0.0
512. C6H7#+R1H=C6H6#+H2	3.30E+12	0.0	0.0
513. C6H7#+R2OH=C6H6#+H2O	1.00E+13	0.0	0.0
514. C6H7#+R4CH3=C6H6#+CH4	3.00E+12	-0.3	-100.0
515. C6H7#+C6H7#=C6H6#+C6H8#	8.40E+10	0.0	-300.0
516. C6H5#=lC6H5	5.00E+13	0.0	72500.0
517. lC6H5=2C2H2+R9C2H	2.00E+13	0.0	51000.0
518. lC6H5=lC6H4+R1H	2.00E+12	0.0	41000.0
519. C6H5#+O2=C6H5O#+B1O	2.60E+13	0.0	6100.0
520. C6H5#+O2=OC6H4O+R1H	3.00E+13	0.0	9000.0
521. C6H5#+O2=C6H5O2	2.20E+19	-2.5	0.0
522. C6H5#+C2H2=C6H5#C2H+R1H	4.00E+13	0.0	10100.0
523. C6H5#+B1O=C5H5#+B2CO	1.00E+14	0.0	0.0
524. C6H5#+R2OH=C6H5OH#	1.00E+13	0.0	0.0
525. C6H5#+R5CHO=C6H5CHO	1.50E+13	0.0	0.0
526. C6H5#+R9C2H=C6H5#C2H	2.54E+17	-1.5	1541.0
527. C6H5#+R10C2H3V=styrene	1.50E+13	0.0	0.0
528. C6H5#+R11C2H5=etC6H5	1.50E+13	0.0	0.0
529. C6H5#+R3OOH=C6H5O#+R2OH	1.50E+13	0.0	0.0
530. C6H5#+C3H3=C6H5C3H3	3.00E+12	0.0	0.0
531. C6H5#+C4H2=C6H5#C2H+R9C2H	2.00E+13	0.0	0.0
532. C6H5#+C6H6#=biphenyl+R1H	5.60E+12	-0.1	7500.0
533. C6H5#+C6H5#=biphenyl	3.80E+31	-5.8	7900.0
534. C6H5#+R2OH=C6H5O#+R1H	5.00E+13	0.0	0.0

535. C6H5#+C6H7#=C6H6#+C6H6#	1.00E+12	0.0	0.0
536. C6H5O2=OC6H4O+R1H	2.00E+13	0.0	30000.0
537. C6H5O2=C5H4O#+R5CHO	2.00E+13	0.0	30000.0
538. C6H5O#=B2CO+C5H5#	2.50E+11	0.0	43800.0
539. C6H5O#+R1H=C6H5OH#	2.50E+14	0.0	0.0
540. C6H5O#+R1H=C5H6#+B2CO	1.10E+53	-10.7	41400.0
541. C6H5O#+B1O=OC6H4OH	2.60E+10	0.5	800.0
542. C6H5O#+B1O=OC6H4O+R1H	8.50E+13	0.0	0.0
543. C6H5O#+B1O=C5H5#+CO2	1.00E+13	0.0	0.0
544. OC6H4OH=B2CO+C5H4OH#	7.40E+11	0.0	43800.0
545. C5H5#=lC5H5	1.00E+14	0.0	45500.0
546. lC5H5+R1H=lC5H6	1.00E+14	0.0	0.0
547. lC5H5=C3H3+C2H2	2.00E+13	0.0	50000.0
548. C5H5#+O2=R5CHO+C4H4O	1.20E+19	-2.5	11000.0
549. C5H5#+R1H=C5H6#	1.00E+14	0.0	0.0
550. C5H5#+B1O=C5H4O#+R1H	5.80E+13	0.0	20.0
551. C5H5#+B1O=>2C2H2+R5CHO	3.20E+13	-0.2	440.0
552. C5H5#+R2OH=>C4H6Z2+B2CO	4.00E+14	0.0	4500.0
553. C5H5#+R2OH=C5H5OH#	1.00E+13	0.0	0.0
554. C5H5#+R3OOH=C5H5O#+R2OH	3.00E+12	0.0	0.0
555. C5H5#+R3OOH=>C5H6#+O2	2.50E+09	1.0	3500.0
556. C5H5O#=2C2H2+R5CHO	2.00E+13	0.0	30000.0
557. C5H5O#=C5H4O#+R1H	2.00E+13	0.0	30000.0
558. C5H5O#+R1H=C5H5OH#	1.00E+14	0.0	0.0
559. C5H4OH#+O2=C5H4O#+R3OOH	1.00E+13	0.0	5000.0
560. C5H4OH#+R1H=C5H5OH#	1.00E+14	0.0	0.0
561. C5H4OH#+B1O=CO2+C2H2+R10C2H3V	3.20E+13	-0.2	440.0
562. C5H4OH#+R3OOH=R2OH+CO2+R10C2H3V+C2H2	3.00E+12	0.0	0.0
563. C5H4OH#+R3OOH=>C5H5OH#+O2	2.50E+09	1.0	3500.0
564. C5H4OH#+C6H5O#=C5H4O#+C6H5OH#	1.00E+12	0.0	0.0
565. OC6H4O=>C5H4O#+B2CO	1.00E+12	0.0	40000.0
566. OC6H4O+R1H=>2B2CO+C2H2+R10C2H3V	5.20E+13	0.0	3200.0
567. OC6H4O+R1H=>H2+2B2CO+C2H2+R9C2H	1.60E+06	2.5	9800.0
568. OC6H4O+R2OH=>H2O+2B2CO+C2H2+R9C2H	4.40E+06	2.0	1400.0
569. C6H5OH#=C5H6#+B2CO	1.00E+12	0.0	61200.0
570. C6H5OH#+O2=R3OOH+C6H5O#	1.00E+13	0.0	38900.0
571. C6H5OH#+B1O=OC6H4OH+R1H	1.60E+13	0.0	3400.0
572. C6H5OH#+R1H=C6H5O#+H2	1.20E+14	0.0	12400.0
573. C6H5OH#+B1O=C6H5O#+R2OH	1.30E+13	0.0	2900.0
574. C6H5OH#+R2OH=C6H5O#+H2O	1.40E+08	1.4	-960.0
575. C6H5OH#+R3OOH=C6H5O#+H2O2	1.00E+12	0.0	10000.0
576. C6H5OH#+R4CH3=C6H5O#+CH4	1.80E+11	0.0	7700.0

577. C6H5OH#+C6H5#=C6H5O#+C6H6#	4.90E+12	0.0	4400.0
578. C6H5OH#+C5H5#=C6H5O#+C5H6#	4.90E+11	0.0	9400.0
579. C6H5OH#+C3H5Y=C6H5O#+C3H6Y	4.90E+11	0.0	9400.0
580. C6H5OH#+iC4H5=C6H5O#+C4H6Z2	4.90E+11	0.0	9400.0
581. C6H5OH#+R1H=C6H4OH#+H2	1.70E+14	0.0	16000.0
582. C6H5OH#+B1O=C6H4OH#+R2OH	2.00E+13	0.0	14700.0
583. C6H5OH#+R2OH=C6H4OH#+H2O	1.40E+13	0.0	4600.0
584. C6H5OH#+R3OOH=C6H4OH#+H2O2	4.00E+11	0.0	28900.0
585. C6H5OH#+R4CH3=C6H4OH#+CH4	2.00E+12	0.0	15000.0
586. C6H4OH#+O2=OC6H4OH+B1O	2.10E+13	0.0	6100.0
587. C6H4OH#+R1H=C6H5OH#	1.00E+14	0.0	0.0
588. C5H6#+O2=>C5H5#+R3OOH	1.40E+12	0.0	31600.0
589. C5H6#+R1H=C5H7#	5.20E+13	0.0	3200.0
590. C5H6#+B1O=C5H5O#+R1H	8.90E+12	-0.1	590.0
591. C5H6#+R1H=C5H5#+H2	2.80E+13	0.0	2000.0
592. C5H6#+B1O=C5H5#+R2OH	4.80E+04	2.7	1100.0
593. C5H6#+R2OH=C5H5#+H2O	3.10E+06	2.0	0.0
594. C5H6#+R3OOH=C5H5#+H2O2	1.10E+04	2.6	12900.0
595. C5H6#+R4CH3=C5H5#+CH4	1.80E-01	4.0	0.0
596. C5H6#+C3H5Y=C5H5#+C3H6Y	6.00E+12	0.0	0.0
597. C5H6#+nC4H5=C5H5#+C4H6Z2	6.00E+12	0.0	0.0
598. C5H6#+iC4H5=C5H5#+C4H6Z2	6.00E+12	0.0	0.0
599. C5H7#=>C2H2+C3H5Y	2.00E+13	0.0	35500.0
600. C5H7#+O2=C5H6#+R3OOH	7.90E+11	0.0	5000.0
601. C5H4O#=2C2H2+B2CO	5.70E+32	-6.8	68500.0
602. C5H4O#+R1H=B2CO+nC4H5	2.60E+13	0.0	3200.0
603. C5H4O#+B1O=C4H4+CO2	1.00E+13	0.0	2000.0
604. C5H4O#+R1H=C5H3O#+H2	2.00E+12	0.0	8100.0
605. C5H4O#+B1O=C5H3O#+R2OH	1.40E+13	0.0	14700.0
606. C5H4O#+R2OH=C5H3O#+H2O	1.10E+08	1.4	1400.0
607. C5H3O#=C2H2+B2CO+R9C2H	2.00E+13	0.0	51000.0
608. C5H3O#+O2=CO2+C2H2+R12CHCOZ	9.70E+58	-13.5	38200.0
609. C5H5OH#+R1H=C5H5O#+H2	4.00E+13	0.0	6100.0
610. C5H5OH#+B1O=C5H5O#+R2OH	1.00E+13	0.0	4600.0
611. C5H5OH#+R2OH=C5H5O#+H2O	1.00E+13	0.0	1700.0
612. C5H5OH#+R1H=C5H4OH#+H2	1.40E+13	0.0	2000.0
613. C5H5OH#+B1O=C5H4OH#+R2OH	4.80E+04	2.7	1100.0
614. C5H5OH#+R2OH=C5H4OH#+H2O	1.50E+06	2.0	0.0
615. C4H4O+R1H=>R10C2H3V+CH2COZ	1.30E+13	0.0	3000.0
616. C4H4O+R1H=>C2H4Z+R12CHCOZ	1.30E+13	0.0	3000.0
617. C4H4O+R1H=>sC3H5+B2CO	1.30E+13	0.0	1500.0
618. C4H4O+R2OH=>C2H3CHO+R5CHO	1.40E+12	0.0	-1000.0

619. C4H4O+R2OH=>CO2+C3H5Y	1.40E+12	0.0	-1000.0
620. C4H4O+B1O=>R13CH2CHO+R12CHCOZ	6.00E+04	2.6	-1100.0
621. C4H4O+B1O=>2CH2COZ	6.00E+04	2.6	-1100.0
622. C4H4O+R1H=>C2H2+R12CHCOZ+H2	8.20E+05	2.5	12300.0
623. C4H4O+R1H=>C3H3+B2CO+H2	4.10E+05	2.5	9800.0
624. C4H4O+R2OH=>C2H2+R12CHCOZ+H2O	2.20E+06	2.0	2800.0
625. C4H4O+R2OH=>C3H3+B2CO+H2O	1.10E+06	2.0	1500.0
626. C4H4O+B1O=>C2H2+R12CHCOZ+R2OH	1.20E+11	0.7	8700.0
627. C4H4O+B1O=>C3H3+B2CO+R2OH	6.00E+10	0.7	8700.0
628. C6H5O#+R4CH3=anisole	5.00E+12	0.0	0.0
629. anisole+O2=>HCHO+C6H5#+R3OOH	1.20E+13	0.0	49000.0
630. B1O+anisole=>R2OH+HCHO+C6H5#	5.10E+13	0.0	7850.0
631. anisole+R1H=>H2+HCHO+C6H5#	2.85E+07	2.0	7700.0
632. anisole+R2OH=>H2O+HCHO+C6H5#	2.67E+06	2.0	450.0
633. anisole+R3OOH=>H2O2+HCHO+C6H5#	6.00E+11	0.0	17000.0
634. anisole+R4CH3=>CH4+HCHO+C6H5#	3.00E-01	4.0	8200.0
635. C6H5O#+C2H2=>benzofuran+R1H	1.20E+12	0.0	460.0
636. C6H5O#+C2H4Z=C8H8O#+R1H	1.20E+12	0.0	460.0
637. R1H+C8H7O#=C8H8O#	1.00E+14	0.0	0.0
638. C8H7O#=benzofuran+R1H	3.00E+13	0.0	50000.0
639. R1H+C8H7O#-1=C8H8O#	1.00E+14	0.0	0.0
640. C8H7O#-1=benzofuran+R1H	3.00E+13	0.0	50000.0
641. benzofuran+R2OH=>C6H4CH3+CO2	1.37E+12	0.0	-1040.0
642. benzofuran+R2OH=>C6H5CO+HCHO	1.37E+12	0.0	-1040.0
643. benzofuran+B1O=>C6H5CO+B2CO+R1H	6.00E+04	2.6	-1130.0
644. o-xylene=o-methylbenzyl+R1H	5.00E+15	0.0	88300.0
645. o-xylene=C6H4CH3+R4CH3	4.00E+17	0.0	97000.0
646. o-xylene+O2=o-methylbenzyl+R3OOH	4.20E+12	0.0	38600.0
647. o-xylene+R1H=toluene+R4CH3	1.16E+14	0.0	8100.0
648. o-xylene+B1O=OC6H3(CH3)2+R1H	1.70E+13	0.0	3600.0
649. o-xylene+R2OH=HOC6H3(CH3)2+R1H	1.30E+13	0.0	10600.0
650. o-xylene+R1H=o-methylbenzyl+H2	2.40E+14	0.0	8400.0
651. o-xylene+B1O=o-methylbenzyl+R2OH	1.26E+12	0.0	0.0
652. o-xylene+R2OH=o-methylbenzyl+H2O	1.04E+10	1.0	870.0
653. o-xylene+R3OOH=o-methylbenzyl+H2O2	8.00E+11	0.0	14000.0
654. o-xylene+R4CH3=o-methylbenzyl+CH4	3.20E+12	0.0	11100.0
655. o-xylene+R10C2H3V=o-methylbenzyl+C2H4Z	8.00E+12	0.0	8000.0
656. o-xylene+C3H5Y=o-methylbenzyl+C3H6Y	3.20E+12	0.0	15100.0
657. o-xylene+C3H3=o-methylbenzyl+pC3H4	3.20E+12	0.0	15100.0
658. o-xylene+iC4H5=o-methylbenzyl+C4H6Z2	3.20E+12	0.0	15100.0
659. o-xylene+nC4H5=o-methylbenzyl+C4H6Z2	3.20E+12	0.0	11100.0
660. o-xylene+C5H5#=o-methylbenzyl+C5H6#	3.20E+11	0.0	15100.0

661. o-xylene+C6H5#=o-methylbenzyl+C6H6#	7.90E+13	0.0	12000.0
662. o-xylene+benzyl=o-methylbenzyl+toluene	3.20E+11	0.0	15100.0
663. o-xylene+C6H5O#=o-methylbenzyl+C6H5OH#	3.20E+11	0.0	15100.0
664. o-xylene+OC6H4CH3=o-methylbenzyl+HOC6H4CH3	3.20E+11	0.0	15100.0
665. o-xylene+R1H=phenyl(CH3)2+H2	1.20E+09	1.0	16800.0
666. o-xylene+B1O=phenyl(CH3)2+R2OH	4.10E+13	0.0	14700.0
667. o-xylene+R2OH=phenyl(CH3)2+H2O	3.20E+08	1.4	1450.0
668. o-xylene+R3OOH=phenyl(CH3)2+H2O2	1.10E+13	0.0	28900.0
669. o-xylene+R4CH3=phenyl(CH3)2+CH4	4.10E+12	0.0	15000.0
670. o-methylbenzyl=>C6H6#+R1H+C2H2	6.00E+13	0.0	70000.0
671. o-methylbenzyl=o-xylylene+R1H	5.00E+15	0.0	74200.0
672. o-methylbenzyl+O2=CH3C6H4CH2O+B1O	6.30E+12	0.0	40000.0
673. o-methylbenzyl+O2=o-xylylene+R3OOH	7.20E+13	0.0	16710.0
674. o-methylbenzyl+O2=benzocyclobut+R3OOH	7.20E+13	0.0	16710.0
675. o-methylbenzyl+B1O=C6H4CH3+HCHO	3.50E+13	0.0	0.0
676. o-methylbenzyl+B1O=CH3C6H4CHO+R1H	1.00E+14	0.0	0.0
677. o-methylbenzyl+R2OH=CH3C6H4CH2OH	2.00E+13	0.0	0.0
678. o-methylbenzyl+R3OOH=CH3C6H4CH2OOH	5.00E+12	0.0	0.0
679. 2o-methylbenzyl=o-bibenzyl	2.50E+11	0.4	0.0
680. CH3C6H4CH2CH3=>o-methylbenzyl+R4CH3	6.10E+15	0.0	75120.0
681. o-methylbenzyl+R4CH3=>CH3C6H4CH2CH3	3.00E+13	0.0	0.0
682. o-methylbenzyl+C2H2=>C10H10+R1H	3.20E+11	0.0	7000.0
683. o-methylbenzyl+R1H=benzocyclobut+H2	1.80E+13	0.0	0.0
684. o-methylbenzyl+R2OH=benzocyclobut+H2O	6.00E+12	0.0	0.0
685. phenyl(CH3)2+O2=OC6H3(CH3)2+B1O	2.60E+13	0.0	6100.0
686. phenyl(CH3)2+R1H=o-xylene	1.00E+14	0.0	0.0
687. phenyl(CH3)2+B1O=OC6H3(CH3)2	1.00E+14	0.0	0.0
688. phenyl(CH3)2+R2OH=HOC6H3(CH3)2	1.00E+13	0.0	0.0
689. phenyl(CH3)2+R4CH3=trimetbenz	1.20E+06	2.0	-3700.0
690. phenyl(CH3)2+R3OOH=OC6H3(CH3)2+R2OH	5.00E+12	0.0	0.0
691. phenyl(CH3)2+R1H=o-methylbenzyl+R1H	2.00E+13	0.0	0.0
692. CH3C6H4CH2O=R1H+CH3C6H4CHO	2.00E+13	0.0	27500.0
693. CH3C6H4CH2O=C6H4CH3+HCHO	2.00E+13	0.0	27500.0
694. CH3C6H4CH2O+O2=R3OOH+CH3C6H4CHO	6.00E+10	0.0	1600.0
695. CH3C6H4CH2O+R1H=CH3C6H4CH2OH	2.00E+13	0.0	0.0
696. OC6H3(CH3)2=>R1H+toluene+B2CO	3.00E+11	0.0	43800.0
697. OC6H3(CH3)2=>R4CH3+C6H6#+B2CO	3.00E+11	0.0	43800.0
698. OC6H3(CH3)2+R1H=HOC6H3(CH3)2	1.00E+14	0.0	0.0
699. CH3C6H4CHO+O2=CH3C6H4CO+R3OOH	7.00E+11	0.0	39500.0
700. CH3C6H4CHO+O2=CH2C6H4CHO+R3OOH	2.10E+12	0.0	41000.0
701. CH3C6H4CHO=CH3C6H4CO+R1H	3.98E+15	0.0	83740.0
702. CH3C6H4CHO+R1H=toluene+R5CHO	5.80E+13	0.0	8100.0

703. CH3C6H4CHO+R1H=C6H5CHO+R4CH3	5.80E+13	0.0	8100.0
704. CH3C6H4CHO+R1H=CH3C6H4CO+H2	4.00E+13	0.0	3200.0
705. CH3C6H4CHO+B1O=CH3C6H4CO+R2OH	6.00E+12	0.0	1800.0
706. CH3C6H4CHO+R2OH=CH3C6H4CO+H2O	7.80E+12	0.0	0.0
707. CH3C6H4CHO+R3OOH=CH3C6H4CO+H2O2	3.00E+12	0.0	11000.0
708. CH3C6H4CHO+R4CH3=CH3C6H4CO+CH4	2.00E-06	5.6	1500.0
709. CH3C6H4CHO+R11C2H5=CH3C6H4CO+C2H6	1.30E+12	0.0	7500.0
710. CH3C6H4CHO+C3H5Y=CH3C6H4CO+C3H6Y	1.30E+12	0.0	11500.0
711. CH3C6H4CHO+iC4H5=CH3C6H4CO+C4H6Z2	1.30E+12	0.0	11500.0
712. CH3C6H4CHO+nC4H5=CH3C6H4CO+C4H6Z2	1.30E+12	0.0	7500.0
713. CH3C6H4CHO+benzyl=toluene+CH3C6H4CO	1.30E+11	0.0	11500.0
714. CH3C6H4CHO+o-methylbenzyl=o-xylene+CH3C6H4CO	1.30E+11	0.0	11500.0
715. CH3C6H4CHO+C6H5O#=CH3C6H4CO+C6H5OH#	1.30E+11	0.0	11500.0
716. CH3C6H4CHO+OC6H3(CH3)2=CH3C6H4CO+HOC6H3(CH3)2	1.30E+11	0.0	11500.0
717. CH3C6H4CHO+OC6H4CH3=CH3C6H4CO+HOC6H4CH3	1.30E+11	0.0	11500.0
718. CH3C6H4CHO+C5H5#=CH3C6H4CO+C5H6#	1.30E+11	0.0	11500.0
719. CH3C6H4CHO+HOC6H4CH2=CH3C6H4CO+HOC6H4CH3	1.30E+11	0.0	11500.0
720. CH3C6H4CHO+C6H5#=CH3C6H4CO+C6H6#	1.30E+11	0.0	11500.0
721. CH3C6H4CHO+R1H=CH2C6H4CHO+H2	4.00E+13	0.0	3200.0
722. CH3C6H4CHO+B1O=CH2C6H4CHO+R2OH	6.00E+12	0.0	1800.0
723. CH3C6H4CHO+R2OH=CH2C6H4CHO+H2O	7.80E+12	0.0	0.0
724. CH3C6H4CHO+R3OOH=CH2C6H4CHO+H2O2	3.00E+12	0.0	11000.0
725. CH3C6H4CHO+R4CH3=CH2C6H4CHO+CH4	2.00E-06	5.6	1500.0
726. CH3C6H4CHO+R11C2H5=CH2C6H4CHO+C2H6	1.30E+12	0.0	7500.0
727. CH3C6H4CHO+C3H5Y=CH2C6H4CHO+C3H6Y	1.30E+12	0.0	11500.0
728. CH3C6H4CHO+iC4H5=CH2C6H4CHO+C4H6Z2	1.30E+12	0.0	11500.0
729. CH3C6H4CHO+nC4H5=CH2C6H4CHO+C4H6Z2	1.30E+12	0.0	7500.0
730. CH3C6H4CHO+benzyl=toluene+CH2C6H4CHO	1.30E+11	0.0	11500.0
731. CH3C6H4CHO+o-methylbenzyl=o-xylene+CH2C6H4CHO	1.30E+11	0.0	11500.0
732. CH3C6H4CHO+C6H5O#=CH2C6H4CHO+C6H5OH#	1.30E+11	0.0	11500.0
733. CH3C6H4CHO+OC6H4CH3=CH2C6H4CHO+HOC6H4CH3	1.30E+11	0.0	11500.0
734. CH3C6H4CHO+C5H5#=CH2C6H4CHO+C5H6#	1.30E+11	0.0	11500.0
735. CH3C6H4CHO+HOC6H4CH2=CH2C6H4CHO+HOC6H4CH3	1.30E+11	0.0	11500.0
736. CH3C6H4CHO+C6H5#=CH2C6H4CHO+C6H6#	1.30E+11	0.0	11500.0
737. CH3C6H4CO=C6H4CH3+B2CO	4.00E+14	0.0	29500.0
738. CH2C6H4CHO+O2=CH2OC6H4CHO+B1O	6.30E+12	0.0	40000.0
739. CH2C6H4CHO+R1H=CH3C6H4CHO	1.00E+14	0.0	0.0
740. CH2C6H4CHO+R3OOH=CH2OC6H4CHO+R2OH	5.00E+12	0.0	0.0
741. CH2C6H4CHO+R4CH3=C6H5CHO+C2H4Z	5.00E+12	0.0	0.0
742. CH2OC6H4CHO=>o-phtaldehyde+R1H	2.00E+13	0.0	27500.0
743. CH2OC6H4CHO=C6H4CHO+HCHO	2.00E+13	0.0	27500.0
744. C6H4CHO+R1H=C6H5CHO	1.00E+14	0.0	0.0

745. CH2OC6H4CHO+O2=>R3OOH+o-phtaldehyde	6.00E+10	0.0	1600.0
746. CH3C6H4CH2OOH=CH3C6H4CH2O+R2OH	1.50E+16	0.0	42000.0
747. HOC6H3(CH3)2+O2=OC6H3(CH3)2+R3OOH	1.00E+13	0.0	38900.0
748. HOC6H3(CH3)2+O2=CH3HOC6H3CH2+R3OOH	2.10E+12	0.0	38600.0
749. HOC6H3(CH3)2+R1H=HOC6H4CH3+R4CH3	5.80E+13	0.0	8100.0
750. HOC6H3(CH3)2+R1H=OC6H3(CH3)2+H2	1.20E+14	0.0	12400.0
751. HOC6H3(CH3)2+B1O=OC6H3(CH3)2+R2OH	1.30E+13	0.0	2900.0
752. HOC6H3(CH3)2+R2OH=OC6H3(CH3)2+H2O	1.40E+08	1.4	-960.0
753. HOC6H3(CH3)2+R3OOH=OC6H3(CH3)2+H2O2	1.00E+12	0.0	10000.0
754. HOC6H3(CH3)2+R4CH3=OC6H3(CH3)2+CH4	1.80E+11	0.0	7700.0
755. HOC6H3(CH3)2+C6H5#=OC6H3(CH3)2+C6H6#	4.90E+12	0.0	4400.0
756. HOC6H3(CH3)2+C5H5#=OC6H3(CH3)2+C5H6#	4.90E+11	0.0	9400.0
757. HOC6H3(CH3)2+C3H5Y=OC6H3(CH3)2+C3H6Y	4.90E+11	0.0	9400.0
758. HOC6H3(CH3)2+iC4H5=OC6H3(CH3)2+C4H6Z2	4.90E+11	0.0	9400.0
759. HOC6H3(CH3)2+C6H5O#=OC6H3(CH3)2+C6H5OH#	4.90E+11	0.0	9400.0
760. HOC6H3(CH3)2+o-methylbenzyl=OC6H3(CH3)2+o-xylene	4.90E+11	0.0	9400.0
761. HOC6H3(CH3)2+R1H=CH3HOC6H3CH2+H2	2.40E+14	0.0	8400.0
762. HOC6H3(CH3)2+B1O=CH3HOC6H3CH2+R2OH	1.26E+12	0.0	0.0
763. HOC6H3(CH3)2+R2OH=CH3HOC6H3CH2+H2O	1.04E+10	1.0	870.0
764. HOC6H3(CH3)2+R3OOH=CH3HOC6H3CH2+H2O2	8.00E+11	0.0	14000.0
765. HOC6H3(CH3)2+R4CH3=CH3HOC6H3CH2+CH4	3.20E+12	0.0	11100.0
766. HOC6H3(CH3)2+C3H5Y=CH3HOC6H3CH2+C3H6Y	3.20E+12	0.0	15100.0
767. HOC6H3(CH3)2+C3H3=CH3HOC6H3CH2+pC3H4	3.20E+12	0.0	15100.0
768. HOC6H3(CH3)2+iC4H5=CH3HOC6H3CH2+C4H6Z2	3.20E+12	0.0	15100.0
769. HOC6H3(CH3)2+nC4H5=CH3HOC6H3CH2+C4H6Z2	3.20E+12	0.0	11100.0
770. HOC6H3(CH3)2+C5H5#=CH3HOC6H3CH2+C5H6#	3.20E+11	0.0	15100.0
771. HOC6H3(CH3)2+C6H5#=CH3HOC6H3CH2+C6H6#	1.58E+14	0.0	12000.0
772. HOC6H3(CH3)2+C6H5O#=CH3HOC6H3CH2+C6H5OH#	3.20E+11	0.0	15100.0
773. HOC6H3(CH3)2+o-methylbenzyl=CH3HOC6H3CH2+o-xylene	3.20E+11	0.0	15100.0
774. HOC6H3(CH3)2+C6H4CH3=CH3HOC6H3CH2+toluene	1.58E+14	0.0	12000.0
775. HOC6H3(CH3)2+OC6H4CH3=CH3HOC6H3CH2+HOC6H4CH3	3.20E+11	0.0	15100.0
776. HOC6H3(CH3)2+C6H5CH2O=CH3HOC6H3CH2+C6H5CH2OH	3.20E+11	0.0	11100.0
777. CH3HOC6H3CH2+O2=CH3HOC6H3CH2O+B1O	6.30E+12	0.0	40000.0
778. CH3HOC6H3CH2+R3OOH=CH3HOC6H3CH2O+R2OH	5.00E+12	0.0	0.0
779. CH3HOC6H3CH2+R1H=HOC6H3(CH3)2	1.00E+14	0.0	0.0
780. CH3HOC6H3CH2+R4CH3=HOC6H4CH3+C2H4Z	5.00E+12	0.0	0.0
781. CH3HOC6H3CH2O=R1H+CH3OHC6H3CHO	2.00E+13	0.0	27500.0
782. CH3HOC6H3CH2O=CH3C6H4OH#+HCHO	2.00E+13	0.0	27500.0
783. CH3HOC6H3CH2O+O2=R3OOH+CH3OHC6H3CHO	6.00E+10	0.0	1600.0
784. CH3OHC6H3CHO+R1H=CH3C6H3OHCO+H2	4.00E+13	0.0	3200.0
785. CH3OHC6H3CHO+B1O=CH3C6H3OHCO+R2OH	6.00E+12	0.0	1800.0
786. CH3OHC6H3CHO+R2OH=CH3C6H3OHCO+H2O	7.80E+12	0.0	0.0

787. CH3OHC6H3CHO+R3OOH=CH3C6H3OHCO+H2O2	3.00E+12	0.0	11000.0
788. CH3OHC6H3CHO+R4CH3=CH3C6H3OHCO+CH4	2.00E-06	5.6	1500.0
789. CH3C6H3OHCO=CH3C6H4OH#+B2CO	4.00E+14	0.0	29500.0
790. CH3C6H4OH#+R1H=HOC6H4CH3	1.00E+14	0.0	0.0
791. CH3C6H4CH2OH+O2=R3OOH+CH3C6H4CHOH	1.40E+12	0.0	34000.0
792. CH3C6H4CH2OH+R1H=toluene+R6CH2OH	5.80E+13	0.0	8100.0
793. CH3C6H4CH2OH+R1H=C6H5CH2OH+R4CH3	5.80E+13	0.0	8100.0
794. CH3C6H4CH2OH+R1H=CH3C6H4CHOH+H2	8.00E+13	0.0	6400.0
795. CH3C6H4CH2OH+B1O=CH3C6H4CHOH+R2OH	4.20E+11	0.0	-2000.0
796. CH3C6H4CH2OH+R2OH=CH3C6H4CHOH+H2O	3.50E+09	1.0	-1130.0
797. CH3C6H4CH2OH+R3OOH=CH3C6H4CHOH+H2O2	2.70E+11	0.0	12000.0
798. CH3C6H4CH2OH+R4CH3=CH3C6H4CHOH+CH4	1.10E+12	0.0	9100.0
799. CH3C6H4CH2OH+C3H5Y=CH3C6H4CHOH+C3H6Y	1.10E+12	0.0	13100.0
800. CH3C6H4CH2OH+iC4H5=CH3C6H4CHOH+C4H6Z2	1.10E+12	0.0	13100.0
801. CH3C6H4CH2OH+nC4H5=CH3C6H4CHOH+C4H6Z2	1.11E+00	0.0	13100.0
802. CH3C6H4CH2OH+C6H5#=CH3C6H4CHOH+C6H6#	5.20E+13	0.0	10000.0
803. CH3C6H4CH2OH+C6H4CH3=CH3C6H4CHOH+toluene	5.20E+13	0.0	10000.0
804. CH3C6H4CH2OH+C6H5O#=CH3C6H4CHOH+C6H5OH#	1.10E+11	0.0	13100.0
805. CH3C6H4CH2OH+benzyl=CH3C6H4CHOH+toluene	1.10E+11	0.0	13100.0
806. CH3C6H4CH2OH+o-methylbenzyl=CH3C6H4CHOH+o-xylene	1.10E+11	0.0	13100.0
807. CH3C6H4CH2OH+OC6H4CH3=CH3C6H4CHOH+HOC6H4CH3	1.10E+11	0.0	13100.0
808. CH3C6H4CH2OH+HOC6H4CH2=CH3C6H4CHOH+HOC6H4CH3	1.10E+11	0.0	13100.0
809. CH3C6H4CH2OH+C5H5#=CH3C6H4CHOH+C5H6#	1.10E+11	0.0	13100.0
810. CH3C6H4CHOH=CH3C6H4CHO+R1H	2.00E+14	0.0	23300.0
811. CH3C6H4CH2CH3=R1H+CH3C6H4CHCH3	4.30E+14	0.0	83600.0
812. CH3C6H4CH2CH3+O2=CH3C6H4CHCH3+R3OOH	1.40E+12	0.0	34000.0
813. CH3C6H4CH2CH3+R1H=toluene+R11C2H5	5.80E+13	0.0	8100.0
814. CH3C6H4CH2CH3+R1H=etC6H5+R4CH3	5.80E+13	0.0	8100.0
815. CH3C6H4CH2CH3+R1H=CH3C6H4CHCH3+H2	8.00E+13	0.0	6400.0
816. CH3C6H4CH2CH3+B1O=CH3C6H4CHCH3+R2OH	4.20E+11	0.0	-2.0
817. CH3C6H4CH2CH3+R2OH=CH3C6H4CHCH3+H2O	3.50E+09	1.0	-1130.0
818. CH3C6H4CH2CH3+R3OOH=CH3C6H4CHCH3+H2O2	2.70E+11	0.0	12000.0
819. CH3C6H4CH2CH3+R4CH3=CH3C6H4CHCH3+CH4	1.10E+12	0.0	9100.0
820. CH3C6H4CH2CH3+C3H5Y=CH3C6H4CHCH3+C3H6Y	1.10E+12	0.0	13100.0
821. CH3C6H4CH2CH3+iC4H5=CH3C6H4CHCH3+C4H6Z2	1.10E+12	0.0	13100.0
822. CH3C6H4CH2CH3+nC4H5=CH3C6H4CHCH3+C4H6Z2	1.11E+00	0.0	13100.0
823. CH3C6H4CH2CH3+C6H5O#=CH3C6H4CHCH3+C6H5OH#	1.10E+11	0.0	13100.0
824. CH3C6H4CH2CH3+benzyl=CH3C6H4CHCH3+toluene	1.10E+11	0.0	13100.0
825. CH3C6H4CH2CH3+o-methylbenzyl=CH3C6H4CHCH3+o-xylene	1.10E+11	0.0	13100.0
826. CH3C6H4CH2CH3+OC6H4CH3=CH3C6H4CHCH3+HOC6H4CH3	1.10E+11	0.0	13100.0
827. CH3C6H4CH2CH3+HOC6H4CH2=CH3C6H4CHCH3+HOC6H4CH3	1.10E+11	0.0	13100.0
828. CH3C6H4CH2CH3+C5H5#=CH3C6H4CHCH3+C5H6#	1.10E+11	0.0	13100.0

829. CH3C6H4CHCH3=R1H+CH3styre				3.10E+13	0.0	50670.0
830. CH3C6H4CHCH3+O2=R3OOH+CH3styre				7.00E+11	0.0	15000.0
831. o-bibenzyl=o-C14H13#+R1H				1.00E+16	0.0	83000.0
832. o-bibenzyl+O2=o-C14H13#+R3OOH				2.80E+12	0.0	35000.0
833. o-bibenzyl+R1H=o-C14H13#+H2				1.60E+14	0.0	6400.0
834. o-bibenzyl+B1O=o-C14H13#+R2OH				8.40E+11	0.0	-2.0
835. o-bibenzyl+R2OH=o-C14H13#+H2O				7.00E+09	1.0	-1130.0
836. o-bibenzyl+R3OOH=o-C14H13#+H2O2				5.40E+11	0.0	12000.0
837. o-bibenzyl+R4CH3=o-C14H13#+CH4				2.20E+12	0.0	9100.0
838. o-bibenzyl+C6H5O#=o-C14H13#+C6H5OH#				2.20E+12	0.0	13100.0
839. o-bibenzyl+benzyl=o-C14H13#+toluene				2.20E+12	0.0	13100.0
840. o-bibenzyl+o-methylbenzyl=o-C14H13#+o-xylene				2.20E+12	0.0	13100.0
841. o-bibenzyl+C3H5Y=o-C14H13#+C3H6Y				2.20E+12	0.0	13100.0
842. o-C14H13#=o-stilbene+R1H				7.10E+14	0.0	30000.0
843. o-xylylene=benzocyclobut				2.10E+12	0.0	26830.0
844. benzocyclobut=styrene				1.20E+15	0.0	74320.0
845. benzocyclobut+R1H=>C8H9#-1				1.16E+14	0.0	8100.0
846. benzocyclobut+O2=C6H5C2H2+R3OOH				2.80E+12	0.0	35960.0
847. o-xylylene+B1O=CH2C6H4CHO+R1H				6.00E+08	1.4	900.0
848. C10H10+R2OH=C10H9+H2O				5.00E+06	2.0	0.0
849. C10H10+R1H=C10H9+H2				2.00E+05	2.5	2500.0
850. C10H10+B1O=C10H9+R2OH				7.00E+11	0.7	6000.0
851. naphthalene+R1H=C10H9				5.00E+14	0.0	5000.0
852. C5H4O#=B2CO+C4H4				1.00E+12	0.0	53000.0
853. R1H+R1H+M=H2+M				1.87E+18	-1.0	0.0
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			
	CO2	Enhanced by	1.500E+00			
	H2O	Enhanced by	6.500E+00			
	CH4	Enhanced by	3.000E+00			
	H2	Enhanced by	0.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	3.500E-01			
854. B6CH2+M=B5CH2+M				1.51E+13	0.0	0.0
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			
	CO2	Enhanced by	1.500E+00			
	H2O	Enhanced by	6.500E+00			
	CH4	Enhanced by	4.800E-01			
	C2H4Z	Enhanced by	1.600E+00			
855. B6CH2+R1H=B4CH+H2				3.00E+13	0.0	0.0
856. B5CH2+R1H=B4CH+H2				6.00E+12	0.0	-1800.0

857. B5CH2+B5CH2=>C2H2+R1H+R1H				1.20E+14	0.0	800.0
858. R4CH3+M=B5CH2+R1H+M				2.91E+16	0.0	90700.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
859. R4CH3+R1H=B6CH2+H2				6.00E+13	0.0	15000.0
860. R4CH3+B4CH=R10C2H3V+R1H				3.00E+13	0.0	0.0
861. R4CH3+B6CH2=C2H4Z+R1H				1.80E+13	0.0	0.0
862. R4CH3+B5CH2=C2H4Z+R1H				4.20E+13	0.0	0.0
863. R4CH3+R4CH3(+M)=>C2H6(+M)				3.61E+13	0.0	0.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.36300E+42	-0.70000E+01	0.27600E+04			
TROE centering:	0.62000E+00	0.73000E+02	0.11800E+04			
864. C2H6(+M)=>R4CH3+R4CH3(+M)				1.80E+21	-1.2	90900.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.18900E+50	-0.82400E+01	0.93700E+05			
TROE centering:	0.62000E+00	0.73000E+02	0.11800E+04			
865. R4CH3+R4CH3=R11C2H5+R1H				3.00E+13	0.0	13500.0
866. R4CH3+R4CH3=C2H4Z+H2				2.10E+14	0.0	19300.0
867. R1H+R4CH3(+M)=>CH4(+M)				1.67E+14	0.0	0.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				

AR	Enhanced by	3.500E-01				
Low pressure limit:	0.14080E+25	-0.18000E+01	0.00000E+00			
TROE centering:	0.37000E+00	0.33150E+04	0.61000E+02			
868. CH4(+M)=>R4CH3+R1H(+M)				2.40E+16	0.0	105000.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	0.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.12900E+19	0.00000E+00	0.90900E+05			
TROE centering:	0.00000E+00	0.13500E+04	0.10000E+01	0.78300E+04		
869. CH4(+CH4)=>R4CH3+R1H(+CH4)				2.40E+16	0.0	105000.0
Low pressure limit:	0.84300E+18	0.00000E+00	0.90900E+05			
TROE centering:	0.69000E+00	0.90000E+02	0.22100E+04			
870. CH4+R1H=R4CH3+H2				1.30E+04	3.0	8000.0
871. CH4+B4CH=C2H4Z+R1H				3.00E+13	0.0	-400.0
872. CH4+B6CH2=R4CH3+R4CH3				4.20E+13	0.0	0.0
873. R9C2H+B6CH2=C2H2+B4CH				1.80E+13	0.0	0.0
874. R9C2H+B5CH2=C2H2+B4CH				1.80E+13	0.0	0.0
875. R9C2H+CH4=C2H2+R4CH3				1.20E+12	0.0	0.0
876. C2H2+M=R9C2H+R1H+M				1.14E+17	0.0	107000.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
877. C2H2+R1H=R9C2H+H2				6.60E+13	0.0	27700.0
878. R10C2H3V(+M)=C2H2+R1H(+M)				2.00E+14	0.0	39800.0
O2	nhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.11900E+43	-0.75000E+01	0.45550E+05			
TROE centering:	0.35000E+00	0.10000E+01	0.10000E+09			
879. R10C2H3V+R1H=C2H2+H2				1.20E+13	0.0	0.0
880. R10C2H3V+B6CH2=C2H2+R4CH3				1.80E+13	0.0	0.0

881. R10C2H3V+B5CH2=C2H2+R4CH3					1.80E+13	0.0	0.0
882. R10C2H3V+R4CH3=CH4+C2H2					3.90E+11	0.0	0.0
883. R10C2H3V+R9C2H=2C2H2					9.60E+11	0.0	0.0
884. R10C2H3V+R10C2H3V=C2H4Z+C2H2					9.60E+11	0.0	0.0
885. C2H4Z+M=C2H2+H2+M					9.97E+16	0.0	71600.0
	O2	Enhanced by	4.000E-01				
	B2CO	Enhanced by	7.500E-01				
	CO2	Enhanced by	1.500E+00				
	H2O	Enhanced by	6.500E+00				
	CH4	Enhanced by	3.000E+00				
	C2H6	Enhanced by	3.000E+00				
	AR	Enhanced by	3.500E-01				
886. C2H4Z+M=R10C2H3V+R1H+M					7.40E+17	0.0	96700.0
	O2	Enhanced by	4.000E-01				
	B2CO	Enhanced by	7.500E-01				
	CO2	Enhanced by	1.500E+00				
	H2O	Enhanced by	6.500E+00				
	CH4	Enhanced by	3.000E+00				
	C2H6	Enhanced by	3.000E+00				
	AR	Enhanced by	3.500E-01				
887. C2H4Z+R1H=R10C2H3V+H2					5.00E+07	1.9	13000.0
888. C2H4Z+R4CH3=CH4+R10C2H3V					6.30E+11	0.0	16000.0
889. R11C2H5(+M)=C2H4Z+R1H(+M)					8.20E+13	0.0	40000.0
	O2	Enhanced by	4.000E-01				
	B2CO	Enhanced by	7.500E-01				
	CO2	Enhanced by	1.500E+00				
	H2O	Enhanced by	6.500E+00				
	CH4	Enhanced by	3.000E+00				
	C2H6	Enhanced by	3.000E+00				
	AR	Enhanced by	3.500E-01				
	Low pressure limit:	0.34000E+18	0.00000E+00	0.33400E+05			
	TROE centering:	0.75000E+00	0.97000E+02	0.13790E+04			
890. R11C2H5+R1H=C2H4Z+H2					1.80E+12	0.0	0.0
891. R11C2H5+R1H=C2H6					3.60E+13	0.0	0.0
892. R11C2H5+B6CH2=C2H4Z+R4CH3					9.00E+12	0.0	0.0
893. R11C2H5+B5CH2=C2H4Z+R4CH3					1.80E+13	0.0	0.0
894. R11C2H5+R4CH3=C2H4Z+CH4					1.10E+12	0.0	0.0
895. R11C2H5+R9C2H=C2H2+C2H4Z					1.80E+12	0.0	0.0
896. R11C2H5+R10C2H3V=2C2H4Z					4.80E+11	0.0	0.0
897. R11C2H5+R10C2H3V=C2H2+C2H6					4.80E+11	0.0	0.0
898. R11C2H5+R11C2H5=C2H4Z+C2H6					1.40E+12	0.0	0.0
899. C2H6+M=C2H4Z+H2+M					2.30E+17	0.0	67400.0

900. C2H6+R1H=R11C2H5+H2	1.40E+09	1.5	7400.0
901. C2H6+B6CH2=R4CH3+R11C2H5	1.10E+14	0.0	0.0
902. C2H6+R4CH3=R11C2H5+CH4	1.50E-07	6.0	5800.0
903. C2H6+R9C2H=C2H2+R11C2H5	3.60E+12	0.0	0.0
904. C2H6+R10C2H3V=R11C2H5+C2H4Z	6.00E+02	3.3	10500.0
905. B1O+H2=R2OH+R1H	5.10E+04	2.7	6200.0
906. B1O+B4CH=B2CO+R1H	3.90E+13	0.0	0.0
907. B1O+B6CH2=>B2CO+2R1H	1.50E+13	0.0	0.0
908. B1O+B6CH2=B2CO+H2	1.50E+13	0.0	0.0
909. B1O+B5CH2=>B2CO+2R1H	7.20E+13	0.0	0.0
910. B1O+B5CH2=B2CO+H2	4.80E+13	0.0	0.0
911. B1O+R4CH3=HCHO+R1H	8.40E+13	0.0	0.0
912. B1O+R4CH3=R7CH3O	8.00E+15	-2.1	600.0
913. B1O+CH4=R4CH3+R2OH	7.20E+08	1.6	8400.0
914. B1O+R9C2H=B4CH+B2CO	1.00E+13	0.0	0.0
915. B1O+C2H2=B5CH2+B2CO	2.17E+06	2.1	1600.0
916. B1O+C2H2=R12CHCOZ+R1H	5.06E+06	2.1	1600.0
917. C2H2+B1O=R9C2H+R2OH	3.16E+15	-0.6	15000.0
918. B1O+R10C2H3V=R4CH3+B2CO	3.00E+13	0.0	0.0
919. B1O+R10C2H3V=CH2COZ+R1H	3.00E+13	0.0	0.0
920. B1O+C2H4Z=HCHO+B5CH2	4.00E+05	1.9	200.0
921. B1O+C2H4Z=CH2COZ+H2	6.60E+05	1.9	200.0
922. C2H4Z+B1O=R4CH3+R5CHO	3.90E+12	0.0	1494.0
Declared duplicate reaction...			
923. C2H4Z+B1O=R4CH3+R5CHO	6.20E+13	0.0	6855.0
Declared duplicate reaction...			
924. C2H4Z+B1O=R13CH2CHO+R1H	1.70E+12	0.0	1494.0
Declared duplicate reaction...			
925. C2H4Z+B1O=R13CH2CHO+R1H	2.80E+13	0.0	6855.0
Declared duplicate reaction...			
926. B1O+C2H4Z=R2OH+R10C2H3V	1.50E+07	1.9	3700.0
927. B1O+R11C2H5=HCHO+R4CH3	1.10E+13	0.0	0.0
928. B1O+R11C2H5=CH3CHO+R1H	5.50E+13	0.0	0.0
929. B1O+R11C2H5=C2H4Z+R2OH	3.00E+13	0.0	0.0
930. B1O+C2H6=R11C2H5+R2OH	1.00E+09	1.5	5800.0
931. R1H+B1O+M=R2OH+M	1.18E+19	-1.0	0.0

O2	Enhanced by	4.000E-01
B2CO	Enhanced by	7.500E-01
CO2	Enhanced by	1.500E+00
H2O	Enhanced by	6.500E+00
CH4	Enhanced by	3.000E+00
C2H6	Enhanced by	3.000E+00

	AR	Enhanced by	3.500E-01			
932. R1H+R2OH+M=H2O+M				5.53E+22	-2.	0.0
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			
	CO2	Enhanced by	1.500E+00			
	H2O	Enhanced by	2.550E+00			
	CH4	Enhanced by	3.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	1.500E-01			
933. R2OH+H2=R1H+H2O				1.00E+08	1.6	3300.0
934. R2OH+B4CH=R5CHO+R1H				3.00E+13	0.0	0.0
935. R2OH+B6CH2=HCHO+R1H				3.00E+13	0.0	0.0
936. R2OH+B5CH2=HCHO+R1H				1.80E+13	0.0	0.0
937. R2OH+R4CH3=B6CH2+H2O				7.20E+13	0.0	2700.0
938. R2OH+R4CH3(+M)=CH3OH(+M)				6.00E+13	0.0	0.0
	Low pressure limit:	0.14000E+45	-0.82000E+01	0.00000E+00		
	TROE centering:	0.82000E+00	0.20000E+03	0.14380E+04		
939. R2OH+R4CH3=HCHO+H2				3.20E+12	-0.5	10800.0
940. R2OH+R4CH3=R7CH3O+R1H				5.70E+12	-0.2	13900.0
941. R2OH+CH4=R4CH3+H2O				1.60E+07	1.8	2700.0
942. R2OH+R9C2H=B5CH2+B2CO				1.80E+13	0.0	0.0
943. R2OH+R9C2H=R12CHCOZ+R1H				2.00E+13	0.0	0.0
944. R2OH+C2H2=R9C2H+H2O				3.38E+07	2.0	14000.0
945. R2OH+C2H2=CH2COZ+R1H				7.50E+06	1.6	2106.0
946. R2OH+C2H2=R4CH3+B2CO				4.80E-04	4.0	-2000.0
947. R2OH+R10C2H3V=C2H2+H2O				3.00E+13	0.0	0.0
948. R2OH+R10C2H3V=CH3CHO				3.00E+13	0.0	0.0
949. C2H4Z+R2OH=R10C2H3V+H2O				1.30E-01	4.2	-860.0
950. C2H4Z+R2OH=R4CH3+HCHO				3.20E+01	2.7	-1172.0
951. C2H4Z+R2OH=CH3CHO+R1H				8.70E-05	4.6	-618.0
952. R2OH+R11C2H5=C2H4Z+H2O				2.40E+13	0.0	0.0
953. R2OH+R11C2H5=>R4CH3+R1H+HCHO				2.40E+13	0.0	0.0
954. R2OH+C2H6=R11C2H5+H2O				7.20E+06	2.0	900.0
955. R2OH+R2OH=H2O+B1O				1.50E+09	1.1	100.0
956. H2O+B4CH=R6CH2OH				5.70E+12	0.0	-800.0
957. H2O+B6CH2=CH3OH				1.80E+13	0.0	0.0
958. B2CO+R4CH3(+M)=R14CH3CO(+M)				5.00E+11	0.0	6900.0
	Low pressure limit:	0.11000E+15	0.00000E+00	0.38000E+04		
	TROE centering:	0.50000E+00	0.10000E+01	0.10000E+09		
959. B2CO+B1O+M=CO2+M				1.54E+15	0.0	3000.0
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			

CO2	Enhanced by	1.500E+00			
H2O	Enhanced by	6.500E+00			
CH4	Enhanced by	3.000E+00			
C2H6	Enhanced by	3.000E+00			
AR	Enhanced by	3.500E-01			
960. B2CO+R2OH=CO2+R1H			9.30E+10	0.0	0.0
Declared duplicate reaction...					
961. B2CO+R2OH=CO2+R1H			7.10E+05	1.8	1133.0
Declared duplicate reaction...					
962. R5CHO+M=R1H+B2CO+M			1.90E+17	-1.0	17000.0
H2	Enhanced by	2.000E+00			
B2CO	Enhanced by	1.500E+00			
CO2	Enhanced by	2.000E+00			
H2O	Enhanced by	6.000E+00			
963. R5CHO+R1H=H2+B2CO			9.00E+13	0.0	0.0
964. R5CHO+R1H=B1O+B5CH2			4.00E+13	0.0	102500.0
965. R5CHO+B6CH2=R4CH3+B2CO			1.80E+13	0.0	0.0
966. R5CHO+B5CH2=R4CH3+B2CO			1.80E+13	0.0	0.0
967. R5CHO+R4CH3=CH4+B2CO			1.20E+14	0.0	0.0
968. R5CHO+R4CH3=CH3CHO			1.80E+13	0.0	0.0
969. R4CH3+HCHO=R5CHO+CH4			7.70E-08	6.1	1970.0
970. R5CHO+R9C2H=C2H2+B2CO			6.00E+13	0.0	0.0
971. R5CHO+R10C2H3V=C2H4Z+B2CO			9.00E+13	0.0	0.0
972. R10C2H3V+HCHO=R5CHO+C2H4Z			5.40E+03	2.8	5900.0
973. R5CHO+R11C2H5=C2H6+B2CO			1.20E+14	0.0	0.0
974. R11C2H5+HCHO=R5CHO+C2H6			5.57E+03	2.8	5860.0
975. R5CHO+B1O=R1H+CO2			3.00E+13	0.0	0.0
976. R5CHO+B1O=R2OH+B2CO			3.00E+13	0.0	0.0
977. R5CHO+R2OH=H2O+B2CO			1.10E+14	0.0	0.0
978. R5CHO+R5CHO=HCHO+B2CO			3.00E+13	0.0	0.0
979. HCHO+M=R5CHO+R1H+M			1.40E+36	-5.5	96800.0
O2	Enhanced by	4.000E-01			
B2CO	Enhanced by	7.500E-01			
CO2	Enhanced by	1.500E+00			
H2O	Enhanced by	6.500E+00			
CH4	Enhanced by	3.000E+00			
C2H6	Enhanced by	3.000E+00			
AR	Enhanced by	3.500E-01			
980. HCHO+M=H2+B2CO+M			3.26E+36	-5.5	96800.0
O2	Enhanced by	4.000E-01			
B2CO	Enhanced by	7.500E-01			
CO2	Enhanced by	1.500E+00			

	H2O	Enhanced by	6.500E+00		
	CH4	Enhanced by	3.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	3.500E-01		
981. HCHO+R1H=R5CHO+H2				1.30E+08	1.6	2100.0
982. HCHO+B4CH=R13CH2CHO				9.60E+13	0.0	-500.0
983. HCHO+B6CH2=R4CH3+R5CHO				1.20E+12	0.0	0.0
984. HCHO+B1O=R5CHO+R2OH				4.10E+11	0.6	2700.0
985. HCHO+R2OH=R5CHO+H2O				3.40E+09	1.2	-400.0
986. R7CH3O+M=HCHO+R1H+M				1.55E+14	0.0	13500.0
	O2	Enhanced by	4.000E-01		
	B2CO	Enhanced by	7.500E-01		
	CO2	Enhanced by	1.500E+00		
	H2O	Enhanced by	6.500E+00		
	CH4	Enhanced by	3.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	3.500E-01		
987. R7CH3O+R1H=HCHO+H2				1.80E+13	0.0	0.0
988. R7CH3O+B6CH2=R4CH3+HCHO				1.80E+13	0.0	0.0
989. R7CH3O+B5CH2=R4CH3+HCHO				1.80E+13	0.0	0.0
990. R7CH3O+R4CH3=HCHO+CH4				2.40E+13	0.0	0.0
991. R7CH3O+CH4=R4CH3+CH3OH				1.60E+11	0.0	8800.0
992. R7CH3O+R9C2H=HCHO+C2H2				2.40E+13	0.0	0.0
993. R7CH3O+R10C2H3V=HCHO+C2H4Z				2.40E+13	0.0	0.0
994. R7CH3O+C2H4Z=HCHO+R11C2H5				1.20E+11	0.0	6700.0
995. R7CH3O+R11C2H5=HCHO+C2H6				2.40E+13	0.0	0.0
996. R7CH3O+C2H6=R11C2H5+CH3OH				2.40E+11	0.0	7000.0
997. R7CH3O+B1O=HCHO+R2OH				1.80E+12	0.0	0.0
998. R7CH3O+R2OH=HCHO+H2O				1.80E+13	0.0	0.0
999. R7CH3O+B2CO=R4CH3+CO2				1.60E+13	0.0	11700.0
1000. R7CH3O+R5CHO=CH3OH+B2CO				9.10E+13	0.0	0.0
1001. R7CH3O+HCHO=CH3OH+R5CHO				1.00E+11	0.0	3000.0
1002. R7CH3O+R7CH3O=CH3OH+HCHO				6.00E+13	0.0	0.0
1003. R6CH2OH+M=HCHO+R1H+M				1.26E+16	0.0	30000.0
	O2	Enhanced by	4.000E-01		
	B2CO	Enhanced by	7.500E-01		
	CO2	Enhanced by	1.500E+00		
	H2O	Enhanced by	6.500E+00		
	CH4	Enhanced by	3.000E+00		
	C2H6	Enhanced by	3.000E+00		
	AR	Enhanced by	3.500E-01		
1004. R6CH2OH+R1H=R4CH3+R2OH				9.60E+13	0.0	0.0

1005. R6CH2OH+R1H=HCHO+H2	6.00E+12	0.0	0.0
1006. R6CH2OH+H2=CH3OH+R1H	6.70E+05	2.0	13400.0
1007. R6CH2OH+B6CH2=CH3CHO+R1H	1.80E+13	0.0	0.0
1008. R6CH2OH+B5CH2=C2H4Z+R2OH	2.40E+13	0.0	0.0
1009. R6CH2OH+B5CH2=R4CH3+HCHO	1.20E+12	0.0	0.0
1010. R6CH2OH+R4CH3=CH4+HCHO	2.40E+12	0.0	0.0
1011. R6CH2OH+CH4=CH3OH+R4CH3	2.17E+01	3.1	16200.0
1012. R6CH2OH+R9C2H=C2H2+HCHO	4.80E+13	0.0	0.0
1013. R6CH2OH+C2H2=R10C2H3V+HCHO	7.20E+11	0.0	9000.0
1014. R6CH2OH+R10C2H3V=C2H4Z+HCHO	4.20E+13	0.0	0.0
1015. R6CH2OH+R11C2H5=C2H4Z+CH3OH	2.40E+12	0.0	0.0
1016. R6CH2OH+R11C2H5=C2H6+HCHO	2.40E+12	0.0	0.0
1017. R6CH2OH+C2H6=CH3OH+R11C2H5	1.99E+02	3.0	14000.0
1018. R6CH2OH+B1O=HCHO+R2OH	4.20E+13	0.0	0.0
1019. R6CH2OH+R2OH=H2O+HCHO	2.40E+13	0.0	0.0
1020. R6CH2OH+R5CHO=CH3OH+B2CO	1.20E+14	0.0	0.0
1021. R6CH2OH+R5CHO=HCHO+HCHO	1.80E+14	0.0	0.0
1022. R6CH2OH+HCHO=CH3OH+R5CHO	5.50E+03	2.8	5900.0
1023. R6CH2OH+R7CH3O=CH3OH+HCHO	2.40E+13	0.0	0.0
1024. R6CH2OH+R6CH2OH=CH3OH+HCHO	1.40E+13	0.0	0.0
1025. CH3OH+R1H=R4CH3+H2O	2.00E+14	0.0	5300.0
1026. CH3OH+R1H=R7CH3O+H2	4.20E+06	2.1	4900.0
1027. CH3OH+B6CH2=R6CH2OH+R4CH3	1.50E+12	0.0	0.0
1028. CH3OH+B5CH2=R4CH3+R6CH2OH	3.19E+01	3.2	7200.0
1029. CH3OH+B5CH2=R4CH3+R7CH3O	1.44E+01	3.1	6900.0
1030. CH3OH+R9C2H=C2H2+R6CH2OH	6.00E+12	0.0	0.0
1031. CH3OH+R9C2H=C2H2+R7CH3O	1.20E+12	0.0	0.0
1032. CH3OH+R10C2H3V=C2H4Z+R6CH2OH	3.19E+01	3.2	7200.0
1033. CH3OH+R10C2H3V=C2H4Z+R7CH3O	1.44E+01	3.1	6900.0
1034. CH3OH+B1O=R6CH2OH+R2OH	3.40E+13	0.0	5500.0
1035. CH3OH+B1O=R7CH3O+R2OH	1.00E+13	0.0	4700.0
1036. CH3OH+R2OH=R6CH2OH+H2O	3.10E+06	2.0	-340.0
1037. CH3OH+R2OH=R7CH3O+H2O	5.40E+05	2.0	-340.0
1038. CH3OH+R7CH3O=CH3OH+R6CH2OH	3.00E+11	0.0	4100.0
1039. R12CHCOZ+M=B4CH+B2CO+M	6.00E+15	0.0	58800.0
1040. R12CHCOZ+R1H=B5CH2+B2CO	1.50E+14	0.0	0.0
1041. R12CHCOZ+R1H=B6CH2+B2CO	1.30E+14	0.0	0.0
1042. R12CHCOZ+B5CH2=R9C2H+HCHO	1.00E+13	0.0	2000.0
1043. R12CHCOZ+B5CH2=R10C2H3V+B2CO	3.00E+13	0.0	0.0
1044. R12CHCOZ+B1O=>B2CO+B2CO+R1H	9.60E+13	0.0	0.0
1045. R12CHCOZ+R2OH=>R5CHO+B2CO+R1H	1.00E+13	0.0	0.0
1046. CH2COZ+M=R12CHCOZ+R1H+M	2.70E+17	0.0	87000.0

O2	Enhanced by	4.000E-01
B2CO	Enhanced by	7.500E-01
CO2	Enhanced by	1.500E+00
H2O	Enhanced by	6.500E+00
CH4	Enhanced by	3.000E+00
C2H6	Enhanced by	3.000E+00
AR	Enhanced by	3.500E-01

1047. CH2COZ+R1H=R4CH3+B2CO	3.30E+10	0.9	2840.0
1048. CH2COZ+R1H=R12CHCOZ+H2	5.00E+13	0.0	8000.0
1049. CH2COZ+B5CH2=C2H4Z+B2CO	1.30E+14	0.0	0.0
1050. CH2COZ+B1O=B5CH2+CO2	1.80E+12	0.0	1300.0
1051. CH2COZ+B1O=R12CHCOZ+R2OH	1.00E+13	0.0	8000.0
1052. CH2COZ+R2OH=R12CHCOZ+H2O	7.50E+12	0.0	2000.0
1053. CH2COZ+R2OH=R4CH3+CO2	6.70E+11	0.0	-1013.0
1054. CH2COZ+R2OH=R6CH2OH+B2CO	1.00E+12	0.0	-1013.0
1055. R14CH3CO+R1H=R4CH3+R5CHO	9.60E+13	0.0	0.0
1056. R14CH3CO+B6CH2=R4CH3+CH2COZ	1.80E+13	0.0	0.0
1057. R14CH3CO+B5CH2=R4CH3+CH2COZ	1.80E+13	0.0	0.0
1058. R14CH3CO+B1O=R4CH3+CO2	9.60E+12	0.0	0.0
1059. R14CH3CO+R2OH=CH2COZ+H2O	1.20E+13	0.0	0.0
1060. R14CH3CO+R2OH=>R4CH3+B2CO+R2OH	3.00E+13	0.0	0.0
1061. R14CH3CO+R5CHO=CH3CHO+B2CO	9.00E+12	0.0	0.0
1062. R14CH3CO+HCHO=CH3CHO+R5CHO	1.80E+11	0.0	12900.0
1063. R14CH3CO+R7CH3O=CH3OH+CH2COZ	6.00E+12	0.0	0.0
1064. R14CH3CO+R7CH3O=HCHO+CH3CHO	6.00E+12	0.0	0.0
1065. R14CH3CO+CH3OH=CH3CHO+R6CH2OH	4.85E+03	3.0	12300.0
1066. R14CH3CO+R14CH3CO=CH2COZ+CH3CHO	1.20E+13	0.0	0.0
1067. R13CH2CHO=R14CH3CO	1.00E+13	0.0	47000.0
1068. R13CH2CHO=R1H+CH2COZ	2.40E+25	-4.8	43424.0
1069. R13CH2CHO=R4CH3+B2CO	1.20E+30	-6.1	41332.0
1070. R13CH2CHO+R1H=R4CH3+R5CHO	1.00E+14	0.0	0.0
1071. R13CH2CHO+R1H=R14CH3CO+R1H	3.00E+13	0.0	0.0
1072. R13CH2CHO+R1H=CH2COZ+H2	2.00E+13	0.0	0.0
1073. R13CH2CHO+B1O=CH2COZ+R2OH	5.00E+13	0.0	0.0
1074. R13CH2CHO+R2OH=CH2COZ+H2O	2.00E+13	0.0	0.0
1075. R13CH2CHO+R2OH=R6CH2OH+R5CHO	1.00E+13	0.0	0.0
1076. R13CH2CHO+O2=HCHO+B2CO+R2OH	5.70E+17	-1.8	11067.0
1077. R13CH2CHO+R3OOH=HCHO+R5CHO+R2OH	7.00E+12	-0.5	0.0
1078. R13CH2CHO+R3OOH=CH3CHO+O2	3.00E+12	-0.5	0.0
1079. R13CH2CHO+B5CH2=C2H4Z+R5CHO	5.00E+13	0.0	0.0
1080. R13CH2CHO+B4CH=R10C2H3V+R5CHO	1.00E+14	0.0	0.0
1081. CH3CHO+R1H=H2+R14CH3CO	4.00E+13	0.0	4200.0

1082. CH3CHO+R4CH3=R14CH3CO+CH4					2.00E-06	5.6	2500.0
1083. CH3CHO+R10C2H3V=C2H4Z+R14CH3CO					8.10E+10	0.0	3700.0
1084. CH3CHO+R11C2H5=C2H6+R14CH3CO					1.30E+12	0.0	8500.0
1085. CH3CHO+B1O=R14CH3CO+R2OH					1.40E+13	0.0	2300.0
1086. CH3CHO+R2OH=R14CH3CO+H2O					4.20E+12	0.0	500.0
1087. CH3CHO+R7CH3O=R14CH3CO+CH3OH					2.40E+11	0.0	1800.0
1088. CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO					2.50E+07	0.0	0.0
1089. C2H4O#3=CH4+B2CO					1.20E+13	0.0	57200.0
1090. C2H4O#3=CH3CHO					7.30E+13	0.0	57200.0
1091. C2H4O#3=R4CH3+R5CHO					3.60E+13	0.0	57200.0
1092. C2H4O#3+R1H=H2+R13CH2CHO					2.00E+13	0.0	8300.0
1093. C2H4O#3+R1H=H2O+R10C2H3V					5.00E+09	0.0	5000.0
1094. C2H4O#3+R1H=C2H4Z+R2OH					9.50E+10	0.0	5000.0
1095. C2H4O#3+R4CH3=CH4+R13CH2CHO					1.10E+12	0.0	11800.0
1096. C2H4O#3+R4CH3=R11C2H5+HCHO					1.40E+11	0.0	7600.0
1097. C2H4O#3+R4CH3=C2H4Z+R7CH3O					1.50E+10	0.0	7600.0
1098. C2H4O#3+R9C2H=C2H2+R13CH2CHO					1.20E+12	0.0	9800.0
1099. C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO					2.00E+12	0.0	9300.0
1100. C2H4O#3+R11C2H5=C2H6+R13CH2CHO					6.80E+11	0.0	11400.0
1101. C2H4O#3+B1O=R2OH+R13CH2CHO					1.90E+12	0.0	5200.0
1102. C2H4O#3+R2OH=H2O+R13CH2CHO					1.80E+13	0.0	3600.0
1103. C2H4O#3+R5CHO=HCHO+R13CH2CHO					3.70E+12	0.0	15800.0
1104. C2H4O#3+R7CH3O=CH3OH+R13CH2CHO					1.30E+12	0.0	5800.0
1105. C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO					8.40E+11	0.0	13400.0
1106. C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO					4.00E+12	0.0	17500.0
1107. C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO					6.80E+11	0.0	15400.0
1108. R15C2H5O=HCHO+R4CH3					8.00E+13	0.0	21500.0
1109. R15C2H5O=CH3CHO+R1H					2.00E+14	0.0	23300.0
1110. C2H5OH(+M)=R11C2H5+R2OH(+M)					1.20E+23	-1.5	96000.0
Low pressure limit:	0.32000E+86	-0.18810E+02	0.11490E+06				
TROE centering:	0.50000E+00	0.30000E+03	0.90000E+03	0.50000E+04			
CO2	Enhanced by	3.000E+00					
H2O	Enhanced by	5.000E+00					
B2CO	Enhanced by	2.000E+00					
H2	Enhanced by	2.000E+00					
1111. C2H5OH(+M)=C2H4Z+H2O(+M)					2.80E+13	0.1	66100.0
Low pressure limit:	0.26000E+84	-0.18850E+02	0.86500E+05				
TROE centering:	0.70000E+00	0.35000E+03	0.80000E+03	0.38000E+04			
H2O	Enhanced by	5.000E+00					
1112. C2H5OH(+M)=CH3CHO+H2(+M)					7.20E+11	0.1	91000.0
Low pressure limit:	0.45000E+88	-0.19420E+02	0.11560E+06				
TROE centering:	0.90000E+00	0.90000E+03	0.11000E+04	0.35000E+04			

	H2O	Enhanced by	5.000E+00			
1113. C2H5OH+R1H=H2+R15C2H5O				1.50E+07	1.6	3040.0
1114. C2H5OH+B1O=R2OH+R15C2H5O				1.60E+07	2.0	4450.0
1115. C2H5OH+R2OH=H2O+R15C2H5O				7.50E+11	0.3	1600.0
1116. C2H5OH+R3OOH=H2O2+R15C2H5O				2.50E+12	0.0	24000.0
1117. C2H5OH+R4CH3=CH4+R15C2H5O				1.40E+02	3.0	7650.0
1118. C2H5OH+R1H=H2+R2OH+C2H4Z				1.20E+07	1.8	5100.0
1119. C2H5OH+B1O=R2OH+R2OH+C2H4Z				9.40E+07	1.7	5460.0
1120. C2H5OH+R2OH=H2O+R2OH+C2H4Z				1.70E+11	0.3	600.0
1121. C2H5OH+R3OOH=H2O2+R2OH+C2H4Z				1.20E+04	2.5	15700.0
1122. C2H5OH+R4CH3=CH4+R2OH+C2H4Z				2.20E+02	3.2	9600.0
1123. C2H5OH+R1H=H2+CH3CHO+R1H				2.60E+07	1.6	2800.0
1124. C2H5OH+B1O=R2OH+CH3CHO+R1H				1.90E+07	1.9	1820.0
1125. C2H5OH+R2OH=H2O+CH3CHO+R1H				4.60E+11	0.1	0.0
1126. C2H5OH+R3OOH=H2O2+CH3CHO+R1H				8.20E+03	2.5	10700.0
1127. C2H5OH+R4CH3=CH4+CH3CHO+R1H				7.30E+02	3.0	7900.0
1128. B1O+B1O+M=O2+M				5.40E+13	0.0	-1790.0
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			
	CO2	Enhanced by	1.500E+00			
	H2O	Enhanced by	6.500E+00			
	CH4	Enhanced by	3.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	3.500E-01			
1129. O2+R1H=R2OH+B1O				9.80E+13	0.0	14800.0
1130. O2+R1H(+M)=R3OOH(+M)				4.52E+13	0.0	0.0
	Low pressure limit:	0.18000E+19	-0.80000E+00	0.00000E+00		
	TROE centering:	0.50000E+00	0.10000E+01	0.10000E+09		
	O2	Enhanced by	4.000E-01			
	B2CO	Enhanced by	7.500E-01			
	CO2	Enhanced by	1.500E+00			
	H2O	Enhanced by	0.000E+00			
	CH4	Enhanced by	3.000E+00			
	C2H6	Enhanced by	3.000E+00			
	AR	Enhanced by	2.900E-01			
1131. O2+R1H(+H2O)=R3OOH(+H2O)				4.52E+13	0.0	0.0
	Low pressure limit:	0.69000E+16	0.00000E+00	-0.20800E+04		
	TROE centering:	0.45000E+00	0.10000E+01	0.10000E+09		
1132. O2+B4CH=R5CHO+B1O				3.30E+13	0.0	0.0
1133. O2+B4CH=B2CO+R2OH				3.20E+13	0.0	0.0
1134. O2+B6CH2=>B2CO+R2OH+R1H				3.10E+12	0.0	0.0
1135. O2+B5CH2=R5CHO+R2OH				4.30E+10	0.0	-500.0

1136. O2+B5CH2=CO2+H2				6.90E+11	0.0	500.0
1137. O2+B5CH2=>CO2+R1H+R1H				1.60E+12	0.0	1000.0
1138. O2+B5CH2=B2CO+H2O				1.90E+10	0.0	-1000.0
1139. O2+B5CH2=>B2CO+R2OH+R1H				8.60E+10	0.0	-500.0
1140. O2+B5CH2=HCHO+B1O				1.00E+14	0.0	4500.0
1141. O2+R4CH3(+M)=R8CH3OO(+M)				7.80E+08	1.2	0.0
Low pressure limit:	0.56000E+26	-0.33000E+01	0.00000E+00			
N2	Enhanced by	1.100E+00				
H2O	Enhanced by	1.000E+01				
1142. O2+R4CH3=R7CH3O+B1O				1.30E+14	0.0	31300.0
1143. O2+R4CH3=HCHO+R2OH				3.00E+30	-4.7	36600.0
1144. O2+CH4=R4CH3+R3OOH				4.00E+13	0.0	56700.0
1145. O2+R9C2H=B2CO+R5CHO				3.80E+13	-0.2	0.0
1146. O2+R9C2H=R12CHCOZ+B1O				9.00E+12	-0.2	0.0
1147. O2+C2H2=R9C2H+R3OOH				1.20E+13	0.0	74500.0
1148. O2+C2H2=R5CHO+R5CHO				7.00E+07	1.8	30600.0
1149. O2+R10C2H3V=C2H2+R3OOH				1.34E+06	1.6	-400.0
1150. O2+R10C2H3V=HCHO+R5CHO				4.50E+16	-1.4	1000.0
1151. O2+R10C2H3V=B1O+R13CH2CHO				3.30E+11	-0.3	10.0
1152. O2+C2H4Z=R10C2H3V+R3OOH				4.20E+13	0.0	57400.0
1153. O2+R11C2H5=C2H4Z+R3OOH				8.40E+11	0.0	3900.0
1154. O2+R11C2H5=R15C2H5O+B1O				1.20E+13	-0.2	27900.0
1155. O2+R11C2H5=CH3CHO+R2OH				6.00E+10	0.0	6900.0
1156. O2+C2H6=R11C2H5+R3OOH				6.00E+13	0.0	51700.0
1157. O2+R2OH=R3OOH+B1O				2.20E+13	0.0	52500.0
1158. O2+B2CO=CO2+B1O				2.50E+12	0.0	47700.0
1159. O2+R5CHO=B2CO+R3OOH				7.60E+12	0.0	410.0
1160. O2+HCHO=R5CHO+R3OOH				2.00E+13	0.0	38800.0
1161. O2+R7CH3O=HCHO+R3OOH				2.20E+10	0.0	1700.0
1162. O2+R6CH2OH=HCHO+R3OOH				1.20E+12	0.0	0.0
1163. O2+CH3OH=R6CH2OH+R3OOH				2.00E+13	0.0	44900.0
1164. O2+R12CHCOZ=>B2CO+B2CO+R2OH				1.50E+12	0.0	2500.0
1165. R13CH2CHO+O2=CH2COZ+R3OOH				1.00E+10	0.0	-1400.0
1166. O2+CH3CHO=R14CH3CO+R3OOH				5.00E+13	0.0	36400.0
1167. O2+C2H4O#3=R3OOH+R13CH2CHO				5.00E+13	0.0	48000.0
1168. O2+R15C2H5O=CH3CHO+R3OOH				6.00E+10	0.0	1700.0
1169. R3OOH+R1H=H2+O2				4.30E+13	0.0	1400.0
1170. R3OOH+R1H=2R2OH				1.70E+14	0.0	900.0
1171. R3OOH+R1H=H2O+B1O				3.00E+13	0.0	1700.0
1172. R3OOH+B6CH2=HCHO+R2OH				3.00E+13	0.0	0.0
1173. R3OOH+B5CH2=HCHO+R2OH				1.80E+13	0.0	0.0
1174. R3OOH+R4CH3=R7CH3O+R2OH				1.80E+13	0.0	0.0

1175. R3OOH+CH4=R4CH3+H2O2				9.00E+12	0.0	24600.0
1176. R3OOH+R9C2H=R12CHCOZ+R2OH				1.80E+13	0.0	0.0
1177. R3OOH+C2H2=CH2COZ+R2OH				6.00E+09	0.0	8000.0
1178. R3OOH+R10C2H3V=>R2OH+R4CH3+B2CO				3.00E+13	0.0	0.0
1179. R3OOH+C2H4Z=CH3CHO+R2OH				6.00E+09	0.0	7900.0
1180. R3OOH+C2H4Z=C2H4O#3+R2OH				2.20E+12	0.0	17200.0
1181. R3OOH+R11C2H5=>R4CH3+HCHO+R2OH				2.40E+13	0.0	0.0
1182. R3OOH+R11C2H5=C2H4Z+H2O2				3.00E+11	0.0	0.0
1183. R3OOH+C2H6=R11C2H5+H2O2				1.30E+13	0.0	20400.0
1184. R3OOH+R2OH=H2O+O2				2.90E+13	0.0	-500.0
1185. R3OOH+B2CO=CO2+R2OH				1.50E+14	0.0	23600.0
1186. R3OOH+R5CHO=>R2OH+R1H+CO2				3.00E+13	0.0	0.0
1187. R3OOH+HCHO=R5CHO+H2O2				3.00E+12	0.0	13000.0
1188. R3OOH+R7CH3O=HCHO+H2O2				3.00E+11	0.0	0.0
1189. R3OOH+R6CH2OH=HCHO+H2O2				1.20E+13	0.0	0.0
1190. R3OOH+CH3OH=R6CH2OH+H2O2				9.60E+10	0.0	12600.0
1191. R3OOH+R14CH3CO=>R4CH3+CO2+R2OH				3.00E+13	0.0	0.0
1192. R3OOH+CH3CHO=R14CH3CO+H2O2				1.00E+12	0.0	10000.0
1193. R3OOH+C2H4O#3=H2O2+R13CH2CHO				1.60E+12	0.0	15000.0
1194. R3OOH+R3OOH=H2O2+O2				1.30E+11	0.0	-1630.0
Declared duplicate reaction...						
1195. R3OOH+R3OOH=H2O2+O2				4.20E+14	0.0	11980.0
Declared duplicate reaction...						
1196. R2OH+R2OH(+M)=>H2O2(+M)				7.23E+13	-0.4	0.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.55300E+20	-0.76000E+00	0.00000E+00			
TROE centering:	0.50000E+00	0.10000E+01	0.10000E+09			
1197. H2O2(+M)=>R2OH+R2OH(+M)				3.00E+14	0.0	48500.0
O2	Enhanced by	4.000E-01				
B2CO	Enhanced by	7.500E-01				
CO2	Enhanced by	1.500E+00				
H2O	Enhanced by	6.500E+00				
CH4	Enhanced by	3.000E+00				
C2H6	Enhanced by	3.000E+00				
AR	Enhanced by	3.500E-01				
Low pressure limit:	0.30000E+18	0.00000E+00	0.45500E+05			

TROE centering: 0.50000E+00 0.10000E+01 0.10000E+09

1198.	H2O2+R1H=H2+R3OOH	1.70E+12	0.0	3700.0
1199.	H2O2+R1H=H2O+R2OH	1.00E+13	0.0	3600.0
1200.	H2O2+B6CH2=R7CH3O+R2OH	3.00E+13	0.0	0.0
1201.	H2O2+R10C2H3V=C2H4Z+R3OOH	1.20E+10	0.0	-600.0
1202.	H2O2+B1O=R2OH+R3OOH	6.60E+11	0.0	4000.0
1203.	H2O2+R2OH=H2O+R3OOH	7.80E+12	0.0	1300.0
1204.	CO2+B5CH2=HCHO+B2CO	2.30E+10	0.0	0.0
1205.	R8CH3OO=HCHO+R2OH	1.50E+13	0.0	47000.0
1206.	R8CH3OO+R1H=R7CH3O+R2OH	9.60E+13	0.0	0.0
1207.	R8CH3OO+H2=CH3OOH+R1H	3.00E+13	0.0	26000.0
1208.	R8CH3OO+B6CH2=HCHO+R7CH3O	1.80E+13	0.0	0.0
1209.	R8CH3OO+B5CH2=HCHO+R7CH3O	1.80E+13	0.0	0.0
1210.	R8CH3OO+R4CH3=R7CH3O+R7CH3O	5.00E+12	0.0	-1400.0
1211.	R8CH3OO+CH4=CH3OOH+R4CH3	1.80E+11	0.0	18500.0
1212.	R8CH3OO+R9C2H=R7CH3O+R12CHCOZ	2.40E+13	0.0	0.0
1213.	R8CH3OO+C2H2=CH3OOH+R9C2H	5.60E+11	0.0	24500.0
1214.	R8CH3OO+R10C2H3V=R7CH3O+R13CH2CHO	2.40E+13	0.0	0.0
1215.	R8CH3OO+C2H4Z=R7CH3O+C2H4O#3	1.10E+15	0.0	20000.0
1216.	R8CH3OO+C2H4Z=CH3OOH+R10C2H3V	3.90E+12	0.0	24500.0
1217.	R8CH3OO+R11C2H5=R7CH3O+R15C2H5O	2.40E+13	0.0	0.0
1218.	R8CH3OO+C2H6=CH3OOH+R11C2H5	2.90E+11	0.0	14900.0
1219.	R8CH3OO+B1O=R7CH3O+O2	3.60E+13	0.0	0.0
1220.	R8CH3OO+R2OH=CH3OH+O2	6.00E+13	0.0	0.0
1221.	R8CH3OO+R2OH=R7CH3O+R3OOH	3.00E+12	0.0	0.0
1222.	R8CH3OO+B2CO=R7CH3O+CO2	1.00E+14	0.0	24000.0
1223.	R8CH3OO+R5CHO=>R7CH3O+R1H+CO2	3.00E+13	0.0	0.0
1224.	R8CH3OO+HCHO=CH3OOH+R5CHO	1.00E+12	0.0	12100.0
1225.	R8CH3OO+R7CH3O=HCHO+CH3OOH	3.00E+11	0.0	0.0
1226.	R8CH3OO+R6CH2OH=>R7CH3O+R2OH+HCHO	1.20E+13	0.0	0.0
1227.	R8CH3OO+CH3OH=CH3OOH+R6CH2OH	1.80E+12	0.0	13700.0
1228.	R8CH3OO+CH3OH=CH3OOH+R7CH3O	2.80E+11	0.0	18800.0
1229.	R8CH3OO+CH2COZ=CH3OOH+R12CHCOZ	1.70E+12	0.0	27000.0
1230.	R8CH3OO+R14CH3CO=R4CH3+CO2+R7CH3O	2.40E+13	0.0	0.0
1231.	R8CH3OO+CH3CHO=CH3OOH+R14CH3CO	1.00E+12	0.0	12100.0
1232.	R8CH3OO+CH3CHO=CH3OOH+R13CH2CHO	1.70E+12	0.0	19200.0
1233.	R8CH3OO+C2H4O#3=CH3OOH+R13CH2CHO	2.20E+12	0.0	16000.0
1234.	R8CH3OO+R3OOH=CH3OOH+O2	2.50E+11	0.0	-1600.0
1235.	R8CH3OO+R3OOH=>O2+HCHO+H2O	5.00E+10	0.0	0.0
1236.	R8CH3OO+H2O2=CH3OOH+R3OOH	2.40E+12	0.0	9900.0
1237.	R8CH3OO+R8CH3OO=CH3OH+HCHO+O2	2.50E+10	0.0	-800.0
1238.	R8CH3OO+R8CH3OO=R7CH3O+R7CH3O+O2	2.50E+10	0.0	-800.0

1239. CH3OOH=R7CH3O+R2OH	6.00E+14	0.0	42300.0
1240. CH3OOH+B1O=R8CH3OO+R2OH	2.00E+13	0.0	4800.0
1241. CH3OOH+R2OH=H2O+R8CH3OO	1.80E+12	0.0	-370.0
1242. CH3OOH+R7CH3O=>CH3OH+R2OH+HCHO	1.50E+11	0.0	6500.0
1243. iC3H7+B1O=>C2H6CO+R1H	1.00E+00	0.0	0.0
1244. C2H6CO+O2=>R3OOH+CH2COZ+R4CH3	4.20E+12	0.0	49280.0
1245. C2H6CO+B1O=>CH2COZ+R4CH3+R2OH	1.02E+14	0.0	7850.0
1246. C2H6CO+R1H=>CH2COZ+R4CH3+H2	5.70E+07	2.0	7700.0
1247. C2H6CO+R2OH=>CH2COZ+R4CH3+H2O	5.34E+06	2.0	450.0
1248. C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4	6.00E-01	4.0	8200.0
1249. C2H6CO+R3OOH=>CH2COZ+R4CH3+H2O2	1.20E+12	0.0	17000.0
1250. C2H4Z+R4CH3=>R19C3H7	2.10E+11	0.0	7350.0
1251. R11C2H5+R10C2H3V=>C4H8Y	1.50E+13	0.0	0.0
1252. R5CHO+R11C2H5=>C2H5CHO	1.80E+13	0.0	0.0
1253. R14CH3CO+R4CH3=>C2H6CO	4.00E+15	-0.8	0.0
1254. C2H3CHO+R2OH=CH2CHCO+H2O	1.00E+13	0.0	0.0
1255. C2H3CHO+B1O=CH2CHCO+R2OH	7.20E+12	0.0	2000.0
1256. C2H3CHO+B1O=CH2COZ+R5CHO+R1H	5.00E+07	1.8	80.0
1257. C2H3CHO+R1H=CH2CHCO+H2	4.00E+13	0.0	4200.0
1258. C2H3CHO+R1H=C2H4Z+R5CHO	2.00E+13	0.0	3500.0
1259. C2H3CHO+O2=CH2CHCO+R3OOH	3.00E+13	0.0	36000.0
1260. CH2CHCO=R10C2H3V+B2CO	1.00E+14	0.0	34000.0
1261. CH2CHCO+B1O=R10C2H3V+CO2	1.00E+14	0.0	0.0
1262. C3H5Y+R3OOH=C2H3CHO+R1H+R2OH	7.00E+18	-2.0	0.0
1263. C3H5Y+O2=C2H3CHO+R2OH	1.80E+13	-0.4	22900.0
1264. C3H5Y+B1O=C2H3CHO+R1H	1.80E+14	0.0	0.0
1265. B4CH+C2H2=C3H2+R1H	2.10E+14	0.0	-500.0
1266. C3H2+B1O=R9C2H+R1H+B2CO	3.00E+13	0.0	0.0
1267. C3H2+R2OH=C2H2+R5CHO	5.00E+13	0.0	0.0
1268. C3H2+O2=R12CHCOZ+B2CO+R1H	5.00E+13	0.0	0.0
1269. B6CH2+C2H2=C3H3+R1H	1.80E+14	0.0	0.0
1270. C3H3+R1H=C3H2+H2	2.00E+13	0.0	0.0
1271. C3H3+B1O=R9C2H+HCHO	1.40E+14	0.0	0.0
1272. C3H3+R2OH=C3H2+H2O	2.00E+13	0.0	0.0
1273. C3H3+R2OH=R10C2H3V+R5CHO	4.00E+13	0.0	0.0
1274. C2H2+R12CHCOZ=C3H3+B2CO	1.00E+11	0.0	3000.0
1275. C3H3+O2=CH2COZ+R5CHO	3.00E+10	0.0	2900.0
1276. C3H2+R1H=C3H3	1.00E+14	0.0	0.0
1277. C3H3+R3OOH=R2OH+R9C2H+HCHO	1.00E+15	-0.8	0.0
1278. C3H3+C3H3=C6H5#+R1H	1.00E+12	0.0	0.0
1279. C3H3+C3H3=C6H6#	1.64E+66	-15.9	27529.0
Declared duplicate reaction...			

1280. C3H3+C3H3=C6H6#			1.20E+35	-7.4	5058.0
Declared duplicate reaction...					
1281. pC3H4+M=C3H3+R1H+M			4.70E+18	0.0	80000.0
1282. C2H2+B5CH2=pC3H4			3.50E+12	0.0	0.0
1283. pC3H4=R9C2H+R4CH3			4.20E+15	0.0	125000.0
1284. pC3H4+O2=C3H3+R3OOH			2.10E+12	0.0	40800.0
1285. pC3H4+R1H=C2H2+R4CH3			1.30E+05	2.5	1000.0
1286. pC3H4+R1H(+M)=tC3H5(+M)			8.50E+12	0.0	1700.0
Low pressure limit:	0.56000E+26	-0.72700E+01	0.65800E+04		
1287. pC3H4+R1H(+M)=sC3H5(+M)			5.80E+12	0.0	3100.0
Low pressure limit:	0.38000E+26	-0.72700E+01	0.79800E+04		
1288. pC3H4+R4CH3=C3H3+CH4			2.20E+00	3.5	5700.0
1289. pC3H4+R1H=C3H3+H2			1.70E+05	2.5	2500.0
1290. pC3H4+R9C2H=C3H3+C2H2			3.60E+12	0.0	0.0
1291. pC3H4+R10C2H3V=C3H3+C2H4Z			2.20E+00	3.5	4700.0
1292. pC3H4+R11C2H5=C3H3+C2H6			2.20E+00	3.5	6600.0
1293. pC3H4+B1O=R12CHCOZ+R4CH3			1.50E+13	0.0	2100.0
1294. pC3H4+B1O=R2OH+C3H3			3.40E+04	2.2	4800.0
1295. pC3H4+R2OH=CH2COZ+R4CH3			4.30E+11	0.0	-800.0
1296. pC3H4+R2OH=R1H+C2H3CHO			4.30E+11	0.0	-800.0
1297. pC3H4+R2OH=C3H3+H2O			3.10E+06	2.0	-300.0
1298. pC3H4+R3OOH=C2H4Z+B2CO+R2OH			6.00E+09	0.0	8000.0
1299. pC3H4+R3OOH=C3H3+H2O2			9.60E+03	2.6	13900.0
1300. pC3H4+R7CH3O=CH3OH+C3H3			2.00E+12	0.0	4000.0
1301. pC3H4+C3H3=C6H6#+R1H			1.40E+12	0.0	5000.0
1302. aC3H4=pC3H4			2.50E+12	0.0	59000.0
1303. aC3H4+M=C3H3+R1H+M			2.00E+18	0.0	80000.0
1304. aC3H4+O2=C3H3+R3OOH			2.80E+13	0.0	39000.0
1305. aC3H4+R1H(+M)=C3H5Y(+M)			4.00E+12	0.0	2700.0
Low pressure limit:	0.56000E+34	-0.50000E+01	0.44400E+04		
1306. aC3H4+R1H(+M)=tC3H5(+M)			8.50E+12	0.0	2000.0
Low pressure limit:	0.11000E+35	-0.50000E+01	0.44400E+04		
1307. C2H4Z+B4CH=aC3H4+R1H			1.30E+14	0.0	-300.0
1308. R10C2H3V+B5CH2=aC3H4+R1H			3.00E+13	0.0	0.0
1309. iC4H3+B5CH2=aC3H4+R9C2H			2.00E+13	0.0	0.0
1310. aC3H4+B1O=R1H+B2CO+R10C2H3V			6.60E+12	0.0	3000.0
1311. aC3H4+R2OH=CH2COZ+R4CH3			2.00E+12	0.0	-200.0
1312. aC3H4+R2OH=HCHO+R10C2H3V			2.00E+12	0.0	-200.0
1313. aC3H4+R1H=C3H3+H2			1.30E+06	2.5	9200.0
1314. aC3H4+B1O=C3H3+R2OH			6.20E+12	0.0	1900.0
1315. aC3H4+R2OH=C3H3+H2O			6.20E+06	2.0	400.0
1316. aC3H4+R4CH3=C3H3+CH4			2.00E+12	0.0	7700.0

1317. aC3H4+R9C2H=C3H3+C2H2	1.00E+13	0.0	0.0
1318. aC3H4+C3H5Y=C3H3+C3H6Y	2.00E+12	0.0	7700.0
1319. aC3H4+R7CH3O=CH3OH+C3H3	4.00E+12	0.0	9600.0
1320. aC3H4+R11C2H5=C2H6+C3H3	5.00E+14	0.0	19800.0
1321. aC3H4+R10C2H3V=C2H4Z+C3H3	5.00E+14	0.0	19800.0
1322. aC3H4+R4CH3=iC4H7	4.00E+10	0.0	5000.0
1323. cC3H4=aC3H4	1.50E+14	0.0	50500.0
1324. cC3H4=pC3H4	7.10E+13	0.0	47800.0
1325. cC3H4+R1H=cC3H3+H2	5.40E+04	2.5	-1900.0
1326. cC3H4+R2OH=cC3H3+H2O	3.00E+06	2.0	-1500.0
1327. cC3H4+R2OH=C2H4Z+R5CHO	2.80E+12	0.0	-1000.0
1328. cC3H3+R3OOH=R2OH+C2H2+R5CHO	1.00E+15	-0.8	0.0
1329. cC3H3+R4CH3=cC4H6	1.00E+13	0.0	0.0
1330. cC3H3+R1H=cC3H4	1.00E+14	0.0	0.0
1331. C3H5Y+R1H=aC3H4+H2	1.80E+13	0.0	0.0
1332. C3H5Y+R1H=C3H6Y	1.00E+14	0.0	0.0
1333. C3H5Y+R4CH3=aC3H4+CH4	3.00E+12	-0.3	-100.0
1334. C3H5Y+R4CH3=C4H8Y	1.00E+14	-0.3	-100.0
1335. C3H5Y+R2OH=aC3H4+H2O	6.03E+12	0.0	0.0
1336. C3H5Y+R10C2H3V=aC3H4+C2H4Z	2.40E+12	0.0	0.0
1337. C3H5Y+R11C2H5=aC3H4+C2H6	2.00E+13	0.0	-100.0
1338. C3H5Y+B1O=R10C2H3V+HCHO	1.80E+14	0.0	0.0
1339. C3H5Y+C3H5Y=aC3H4+C3H6Y	8.40E+10	0.0	-300.0
1340. sC3H5=C3H5Y	5.00E+13	0.0	37000.0
1341. R4CH3+C2H2=sC3H5	6.00E+11	0.0	7700.0
1342. tC3H5+R1H=aC3H4+H2	3.30E+12	0.0	0.0
1343. tC3H5+R4CH3=aC3H4+CH4	1.00E+11	0.0	0.0
1344. tC3H5+R10C2H3V=aC3H4+C2H4Z	1.00E+12	0.0	0.0
1345. tC3H5+R11C2H5=aC3H4+C2H6	1.00E+12	0.0	0.0
1346. tC3H5+B1O=CH2COZ+R4CH3	1.80E+14	0.0	0.0
1347. tC3H5+O2=R4CH3+B2CO+HCHO	4.30E+12	0.0	0.0
1348. tC3H5=C3H5Y	2.00E+13	0.0	47000.0
1349. C2H4Z+B6CH2=C3H6Y	9.60E+13	0.0	0.0
1350. C2H4Z+B5CH2=C3H6Y	3.20E+12	0.0	5100.0
1351. R10C2H3V+R4CH3=C3H6Y	2.50E+13	0.0	0.0
1352. C2H4Z+R4CH3=C3H6Y+R1H	6.60E+11	0.0	15900.0
1353. R11C2H5+B6CH2=C3H6Y+R1H	9.00E+12	0.0	0.0
1354. C2H6+B4CH=C3H6Y+R1H	1.10E+14	0.0	-300.0
1355. C3H6Y+R1H=sC3H5+H2	4.60E+05	2.5	9800.0
1356. C3H6Y+R1H=tC3H5+H2	8.00E+05	2.5	12300.0
1357. C3H6Y+R1H=C3H5Y+H2	1.70E+05	2.5	2500.0
1358. C3H6Y+R4CH3=C3H5Y+CH4	2.20E+00	3.5	5700.0

1359. C3H6Y+R4CH3=sC3H5+CH4	8.40E-01	3.5	11700.0
1360. C3H6Y+R4CH3=tC3H5+CH4	1.30E+00	3.5	12900.0
1361. C3H6Y+R11C2H5=C3H5Y+C2H6	2.20E+00	3.5	6600.0
1362. C3H6Y+B1O=C3H5Y+R2OH	1.70E+11	0.7	5900.0
1363. C3H6Y+R2OH=HCHO+R11C2H5	2.90E+12	0.0	-900.0
1364. C3H6Y+R2OH=C3H5Y+H2O	3.10E+06	2.0	-300.0
1365. C3H6Y+R2OH=sC3H5+H2O	1.10E+06	2.0	1450.0
1366. C3H6Y+R2OH=tC3H5+H2O	2.10E+06	2.0	2800.0
1367. C3H6Y+O2=C3H5Y+R3OOH	1.90E+12	0.0	39000.0
1368. C3H6Y+R3OOH=C3H5Y+H2O2	9.60E+03	2.6	13900.0
1369. C3H6Y+R9C2H=pC3H4+R10C2H3V	1.20E+13	0.0	0.0
1370. cC3H6=C3H6Y	4.60E+14	0.0	62600.0
1371. cC3H6+R1H=C3H5Y+H2	1.60E+14	0.0	11700.0
1372. cC3H6+R2OH=C3H5Y+H2O	7.00E+07	1.5	1000.0
1373. cC3H6+R4CH3=C3H5Y+CH4	2.00E+11	0.0	9600.0
1374. nC3H7=R4CH3+C2H4Z	6.40E+12	0.0	31000.0
1375. nC3H7=R1H+C3H6Y	3.00E+13	0.0	38000.0
1376. iC3H7=R1H+C3H6Y	6.00E+13	0.0	39000.0
1377. nC3H7=iC3H7	1.96E+10	1.0	38600.0
1378. nC3H7+O2=R3OOH+C3H6Y	1.60E+12	0.0	5000.0
1379. iC3H7+O2=R3OOH+C3H6Y	1.40E+12	0.0	5000.0
1380. R11C2H5+R4CH3=C3H8	3.40E+13	0.0	0.0
1381. C3H8+O2=>R3OOH+iC3H7	1.40E+13	0.0	50323.7
1382. C3H8+O2=>R3OOH+nC3H7	4.20E+13	0.0	53033.0
1383. B1O+C3H8=>R2OH+iC3H7	2.60E+13	0.0	5200.0
1384. B1O+C3H8=>R2OH+nC3H7	1.00E+14	0.0	7850.0
1385. C3H8+R1H=>H2+iC3H7	9.00E+06	2.0	5000.0
1386. C3H8+R1H=>H2+nC3H7	5.70E+07	2.0	7700.0
1387. C3H8+R2OH=>H2O+iC3H7	2.60E+06	2.0	-765.0
1388. C3H8+R2OH=>H2O+nC3H7	5.40E+06	2.0	450.0
1389. C3H8+R3OOH=>H2O2+iC3H7	4.00E+11	0.0	15500.0
1390. C3H8+R3OOH=>H2O2+nC3H7	1.20E+12	0.0	17000.0
1391. C3H8+R4CH3=>CH4+iC3H7	2.00E+11	0.0	9600.0
1392. C3H8+R4CH3=>CH4+nC3H7	6.00E-01	4.0	8200.0
1393. C3H8+R5CHO=>HCHO+iC3H7	1.00E+07	1.9	17000.0
1394. C3H8+R5CHO=>HCHO+nC3H7	2.00E+05	2.5	18500.0
1395. C3H8+R11C2H5=>C2H6+iC3H7	2.00E+11	0.0	11000.0
1396. C3H8+R11C2H5=>C2H6+nC3H7	6.00E+11	0.0	13500.0
1397. C3H8+iC3H7=>C3H8+nC3H7	8.40E-03	4.2	8700.0
1398. R1H+iC3H7=>C3H8	8.30E+12	0.0	0.0
1399. nC3H7+R1H=C3H8	1.00E+14	0.0	0.0
1400. C4H10+O2=R3OOH+R20C4H9	4.20E+13	0.0	53033.1

1401. C4H10+O2=>R3OOH+R4CH3+C3H6Y				2.80E+13	0.0	50588.3
1402. B1O+C4H10=R2OH+R20C4H9				1.00E+14	0.0	7850.0
1403. B1O+C4H10=>R2OH+R4CH3+C3H6Y				5.20E+13	0.0	5200.0
1404. C4H10+R1H=H2+R20C4H9				5.70E+07	2.0	7700.0
1405. C4H10+R1H=>H2+R4CH3+C3H6Y				1.80E+07	2.0	5000.0
1406. C4H10+R2OH=H2O+R20C4H9				5.40E+06	2.0	450.0
1407. C4H10+R2OH=>H2O+R4CH3+C3H6Y				5.20E+06	2.0	-765.0
1408. C4H10+R3OOH=H2O2+R20C4H9				1.20E+12	0.0	170.0
1409. C4H10+R3OOH=>H2O2+R4CH3+C3H6Y				8.00E+11	0.0	15500.0
1410. C4H10+R4CH3=CH4+R20C4H9				6.00E-01	4.0	8200.0
1411. C4H10+R4CH3=>CH4+R4CH3+C3H6Y				4.00E+11	0.0	9600.0
1412. R9C2H+R9C2H=C4H2				1.80E+13	0.0	0.0
1413. 2C2H2=C4H2+H2				1.50E+13	0.0	42700.0
1414. C2H2+R9C2H=C4H2+R1H				1.82E+14	0.0	467.0
1415. C4H2+R2OH=R5CHO+C3H2				6.70E+12	0.0	-400.0
1416. C4H2+O2=R12CHCOZ+R12CHCOZ				9.60E+12	0.0	31100.0
1417. C4H2+R9C2H=>C6H2+R1H				4.00E+13	0.0	0.0
1418. C6H2+R1H=>C4H2+R9C2H				9.30E+14	0.0	15100.0
1419. nC4H3(+M)=C4H2+R1H(+M)				1.00E+14	0.0	36000.0
Low pressure limit:	0.10000E+15	0.00000E+00	0.30000E+05			
TROE centering:	0.10000E+01	0.10000E+01	0.10000E+09			
1420. C3H3+B4CH=nC4H3+R1H				7.00E+13	0.0	0.0
1421. R9C2H+R10C2H3V=nC4H3+R1H				1.80E+13	0.0	0.0
1422. nC4H3+R1H=iC4H3+R1H				2.40E+11	0.8	2410.0
1423. nC4H3+R1H=C4H2+H2				6.00E+12	0.0	0.0
1424. 2C2H2=nC4H3+R1H				1.00E+12	0.0	64100.0
1425. nC4H3+R2OH=C4H2+H2O				1.50E+13	0.0	0.0
1426. nC4H3+C2H2=C6H4#+R1H				1.64E+09	0.7	12200.0
1427. nC4H3+C2H2=lC6H4+R1H				2.96E+01	3.3	9600.0
1428. nC4H3+C2H2=lC6H5				1.73E+11	-0.4	4000.0
1429. nC4H3+C2H2=C6H5#				3.33E+24	-3.9	9200.0
1430. nC4H3+R10C2H3V=fulvene				4.00E+12	0.0	0.0
1431. nC4H3+R10C2H3V=C6H5#+R1H				1.60E+13	0.0	0.0
1432. nC4H3+R10C2H3V=C4H2+C2H4Z				1.00E+12	0.0	5000.0
1433. nC4H3+R10C2H3V=C4H4+C2H2				2.00E+12	0.0	5000.0
1434. iC4H3=nC4H3				1.50E+13	0.0	67800.0
1435. iC4H3(+M)=C4H2+R1H(+M)				1.00E+14	0.0	55000.0
Low pressure limit:	0.20000E+16	0.00000E+00	0.48000E+05			
TROE centering:	0.10000E+01	0.10000E+01	0.10000E+09			
1436. C3H2+B5CH2=iC4H3+R1H				1.20E+14	0.0	800.0
1437. iC4H3+R1H=2C2H2				2.40E+19	-1.6	2800.0
1438. C3H3+B4CH=iC4H3+R1H				7.00E+13	0.0	0.0

1439. iC4H3+R1H=C4H2+H2	1.20E+13	0.0	0.0
1440. iC4H3+B1O=CH2COZ+R9C2H	2.00E+13	0.0	0.0
1441. iC4H3+R2OH=C4H2+H2O	3.00E+13	0.0	0.0
1442. iC4H3+O2=CH2COZ+R12CHCOZ	1.00E+12	0.0	0.0
1443. iC4H3+R10C2H3V=2C3H3	4.00E+12	0.0	0.0
1444. iC4H3+R10C2H3V=lC6H5+R1H	6.00E+12	0.0	0.0
1445. iC4H3+R10C2H3V=C6H5#+R1H	6.00E+12	0.0	0.0
1446. iC4H3+R10C2H3V=fulvene	1.00E+13	0.0	0.0
1447. iC4H3+R10C2H3V=C4H2+C2H4Z	1.00E+12	0.0	5000.0
1448. iC4H3+R10C2H3V=C4H4+C2H2	2.00E+12	0.0	5000.0
1449. C3H3+B5CH2=C4H4+R1H	4.00E+13	0.0	0.0
1450. R10C2H3V+C2H2=>C4H4+R1H	2.00E+13	0.0	25100.0
1451. C4H4+R1H=>R10C2H3V+C2H2	2.00E+13	0.0	12400.0
1452. C2H4Z+R9C2H=C4H4+R1H	1.20E+13	0.0	0.0
1453. C4H4+R1H=nC4H3+H2	2.00E+07	2.0	15000.0
1454. C4H4+R1H=iC4H3+H2	3.00E+07	2.0	5000.0
1455. R9C2H+C4H4=>C2H2+iC4H3	4.00E+13	0.0	0.0
1456. C2H2+iC4H3=>R9C2H+C4H4	3.00E+13	0.0	27900.0
1457. R10C2H3V+C4H4=>C2H4Z+nC4H3	5.00E+11	0.0	16300.0
1458. nC4H3+C2H4Z=>R10C2H3V+C4H4	3.50E+11	0.0	13400.0
1459. R10C2H3V+C4H4=>C2H4Z+iC4H3	5.00E+11	0.0	16300.0
1460. iC4H3+C2H4Z=>R10C2H3V+C4H4	1.30E+11	0.0	24100.0
1461. C4H4+B1O=aC3H4+B2CO	3.00E+13	0.0	1800.0
1462. C4H4+B1O=pC3H4+B2CO	2.70E+13	0.0	1800.0
1463. C4H4+R2OH=nC4H3+H2O	7.50E+06	2.0	5000.0
1464. C4H4+R2OH=iC4H3+H2O	1.00E+07	2.0	2000.0
1465. aC3H4+aC3H4=C2H4Z+C4H4	1.00E+15	0.0	48000.0
1466. R10C2H3V+C4H4=C6H6#+R1H	1.90E+12	0.0	1250.0
1467. C4H4+C2H2=C6H5#+R1H	1.00E+09	0.0	15000.0
1468. tC4H4+R2OH=iC4H3+H2O	2.00E+07	2.0	2000.0
1469. tC4H4+R1H=iC4H3+H2	3.00E+07	2.0	6000.0
1470. nC4H5(+M)=R1H+C4H4(+M)	1.00E+14	0.0	37000.0
Low pressure limit: 0.10000E+15 0.00000E+00 0.30000E+05			
1471. nC4H5+R1H=C4H4+H2	1.50E+13	0.0	0.0
1472. nC4H5+R1H=iC4H5+R1H	1.00E+14	0.0	0.0
1473. nC4H5+R4CH3=C5H8	1.00E+13	0.0	0.0
1474. nC4H5=C2H2+R10C2H3V	1.00E+14	0.0	43900.0
1475. nC4H5+C2H2=lC6H6+R1H	1.17E-15	7.8	2000.0
1476. nC4H5+C2H2=C6H6#+R1H	1.90E+07	1.5	4200.0
1477. nC4H5+C2H2=fulvene+R1H	2.52E-09	-0.8	4412.0
1478. nC4H5+C2H2=lC6H7	8.74E+12	-1.3	3600.0
1479. nC4H5+C2H2=C6H7#	1.96E+19	-3.4	5200.0

1480. R10C2H3V+nC4H5=lC6H7+R1H	8.28E-28	11.9	5000.0
1481. R10C2H3V+nC4H5=lC6H8	2.90E+15	-0.8	1000.0
1482. R10C2H3V+nC4H5=C6H8#	5.50E+15	-1.7	1500.0
1483. R10C2H3V+nC4H5=C6H6#+H2	2.80E-07	5.6	-1900.0
1484. nC4H5+R2OH=C4H4+H2O	2.50E+12	0.0	0.0
1485. nC4H5+O2=R5CHO+C2H3CHO	4.50E+16	-1.4	1000.0
1486. nC4H5+O2=C4H4+R3OOH	1.34E+06	1.6	-400.0
1487. nC4H5+C4H2=C6H5#C2H+R1H	3.16E+11	0.0	1800.0
1488. nC4H5+R9C2H=fulvene	4.00E+12	0.0	0.0
1489. nC4H5+R9C2H=C6H5#+R1H	1.60E+13	0.0	0.0
1490. nC4H5+R9C2H=C4H4+C2H2	3.00E+12	0.0	5000.0
1491. iC4H5=nC4H5	1.50E+13	0.0	67800.0
1492. iC4H5(+M)=R1H+C4H4(+M)	1.00E+14	0.0	50000.0
Low pressure limit: 0.20000E+16 0.00000E+00 0.42000E+05			
1493. iC4H5+R1H=C4H4+H2	3.00E+13	0.0	0.0
1494. iC4H5+R4CH3=iC5H8	1.00E+13	0.0	0.0
1495. 2R10C2H3V=iC4H5+R1H	1.50E+30	-5.0	13000.0
1496. iC4H5+R2OH=C4H4+H2O	5.50E+12	0.0	0.0
1497. iC4H5+O2=HCHO+CH2CHCO	4.50E+16	-1.4	1000.0
1498. iC4H5+O2=C4H4+R3OOH	1.34E+06	1.6	-400.0
1499. iC4H5+C2H2=C6H6#+R1H	1.47E+23	-3.3	24907.0
1500. iC4H5+C2H2=fulvene+R1H	6.50E+24	-3.4	20319.0
1501. iC4H5+R10C2H3V=C6H6#+H2	1.80E-13	7.1	-1800.0
1502. iC4H5+R9C2H=C6H6#	1.00E+13	0.0	0.0
1503. iC4H5+R9C2H=C6H5#+R1H	6.00E+12	0.0	0.0
1504. iC4H5+R9C2H=fulvene	1.00E+13	0.0	0.0
1505. iC4H5+R9C2H=2C3H3	6.00E+12	0.0	0.0
1506. iC4H5+R9C2H=C4H4+C2H2	3.00E+12	0.0	5000.0
1507. C4H5-1s=R1H+C4H4	6.00E+13	0.0	50400.0
1508. C4H5-1s+R1H=C4H4+H2	2.00E+13	0.0	0.0
1509. C4H5-1s+B1O=R9C2H+CH3CHO	1.40E+14	0.0	0.0
1510. C4H5-1s+R2OH=C4H4+H2O	2.00E+13	0.0	0.0
1511. C4H5-1s+R2OH=R5CHO+sC3H5	4.00E+13	0.0	0.0
1512. C4H5-1s+O2=R5CHO+B2CO+C2H4Z	3.00E+10	0.0	2900.0
1513. C4H5-1s+C4H5-1s=C8H10#	1.00E+12	0.0	0.0
1514. C4H5-1p=R9C2H+C2H4Z	2.00E+14	0.0	57000.0
1515. C4H5-1p+O2=C4H4+R3OOH	1.60E+12	0.0	5000.0
1516. C4H5-1p=C4H5-1s	5.00E+12	0.0	37400.0
1517. C4H5-2=R1H+tC4H4	6.00E+13	0.0	54300.0
1518. C4H5-2=iC4H5	5.00E+12	0.0	50500.0
1519. C4H5-2+C4H5-2=C8H10#	1.00E+12	0.0	0.0
1520. C4H5-2+B1O=C3H3+HCHO	1.40E+14	0.0	0.0

1521. C4H5-2+R2OH=R10C2H3V+B2CO+R4CH3	4.00E+13	0.0	0.0
1522. C4H5-2+O2=CH2COZ+B2CO+R4CH3	3.00E+10	0.0	2900.0
1523. R10C2H3V+R10C2H3V=C4H6Z2	9.80E+14	-0.5	0.0
1524. C4H6Z2=C4H4+H2	2.50E+15	0.0	94700.0
1525. C4H6Z2=iC4H5+R1H	1.40E+15	0.0	98000.0
1526. C2H4Z+R10C2H3V=C4H6Z2+R1H	5.00E+11	0.0	7300.0
1527. C4H6Z2+R1H=nC4H5+H2	1.30E+06	2.5	12200.0
1528. C4H6Z2+R1H=iC4H5+H2	6.60E+05	2.5	9200.0
1529. C4H6Z2+R1H=C4H7-1	2.60E+13	0.0	3200.0
1530. C4H6Z2+R1H=C4H7Y	2.60E+13	0.0	1560.0
1531. C4H6Z2+R4CH3=nC4H5+CH4	7.00E+13	0.0	18500.0
1532. C4H6Z2+R4CH3=iC4H5+CH4	7.00E+13	0.0	15500.0
1533. C4H6Z2+R4CH3=C5H9Y	6.30E+10	0.0	7490.0
1534. C4H6Z2+R4CH3=iC5H9	1.80E+11	0.0	8000.0
1535. C4H6Z2+R10C2H3V=nC4H5+C2H4Z	5.00E+14	0.0	22800.0
1536. C4H6Z2+R10C2H3V=iC4H5+C2H4Z	5.00E+14	0.0	19800.0
1537. C4H6Z2+B1O=C3H5Y+R1H+B2CO	6.00E+08	1.4	900.0
1538. R10C2H3V+C4H6Z2=C6H8#+R1H	7.40E+14	-0.7	8420.0
1539. R10C2H3V+C4H6Z2=lC6H8+R1H	1.00E+10	1.1	14000.0
1540. C4H6Z2+C2H2=C6H8#	2.30E+12	0.0	35000.0
1541. R10C2H3V+C4H6Z2=lC6H9	5.48E+28	-5.3	9300.0
1542. R10C2H3V+C4H6Z2=C6H9Z#	1.64E+29	-6.1	9600.0
1543. C4H6Z2+C2H4Z=C6H10#	2.30E+10	0.0	27000.0
1544. C4H6Z2+R2OH=nC4H5+H2O	6.20E+06	2.0	3400.0
1545. C4H6Z2+R2OH=iC4H5+H2O	3.10E+06	2.0	400.0
1546. C4H6Z2+R2OH=C3H5Y+HCHO	2.80E+12	0.0	-900.0
1547. C4H6Z2+R2OH=CH3CHO+R10C2H3V	5.60E+12	0.0	-900.0
1548. C4H6Z2+O2=iC4H5+R3OOH	4.00E+13	0.0	57900.0
1549. C4H6Z2+C3H3=nC4H5+aC3H4	1.00E+13	0.0	22500.0
1550. C4H6Z2+C3H3=iC4H5+aC3H4	1.00E+13	0.0	19500.0
1551. C4H6-12=C4H6Z2	3.00E+13	0.0	65000.0
1552. C4H6-12=iC4H5+R1H	4.20E+15	0.0	92600.0
1553. C4H6-12+R1H=R10C2H3V+C2H4Z	4.00E+11	0.0	0.0
1554. C4H6-12=C3H3+R4CH3	7.30E+14	0.0	75400.0
1555. C4H6-12+R1H=C4H7-2	1.30E+13	0.0	1600.0
1556. C4H6-12+R1H=C4H7Y	1.20E+11	0.7	3000.0
1557. C4H6-12+R1H=C4H7T	1.30E+13	0.0	3200.0
1558. C4H6-12+R1H=iC4H5+H2	1.70E+05	2.5	2500.0
1559. C4H6-12+R4CH3=iC4H5+CH4	2.20E+00	3.5	5700.0
1560. C4H6-12+R11C2H5=iC4H5+C2H6	2.20E+00	3.5	6600.0
1561. C4H6-12+B1O=iC4H5+R2OH	1.70E+11	0.7	5900.0
1562. C4H6-12+R2OH=iC4H5+H2O	3.10E+06	2.0	-300.0

1563. C4H6-12+R3OOH=iC4H5+H2O2	9.60E+03	2.6	13900.0
1564. B6CH2+pC3H4=cC4H6	1.80E+14	0.0	0.0
1565. cC4H6=C4H6Z2	3.00E+13	0.0	42300.0
1566. cC4H6=C4H6-12	3.00E+13	0.0	43800.0
1567. C4H6-1=C4H6-12	2.50E+13	0.0	65000.0
1568. C4H6-1=C4H5-1s+R1H	7.70E+14	0.0	87900.0
1569. C4H6-1=C4H5-1p+R1H	9.10E+14	0.0	99600.0
1570. C4H6-1=C3H3+R4CH3	2.00E+11	0.0	59500.0
1571. C4H6-1+R1H=R4CH3+aC3H4	3.20E+12	0.0	1700.0
1572. C4H6-1+R1H=R11C2H5+C2H2	3.20E+12	0.0	1700.0
1573. C4H6-1+R1H=H2+C4H5-1s	5.40E+04	2.5	-1900.0
1574. C4H6-1+R4CH3=CH4+C4H5-1s	1.50E+12	0.0	7100.0
1575. C4H6-1+B1O=R2OH+C4H5-1s	8.80E+10	0.7	3200.0
1576. C4H6-1+R2OH=H2O+C4H5-1s	3.00E+06	2.0	-1500.0
1577. C4H6-1+O2=>R3OOH+C4H5-1s	1.40E+12	0.0	41400.0
1578. C4H6-1+R3OOH=>H2O2+C4H5-1s	6.40E+03	2.6	12400.0
1579. C4H6-1+R1H=H2+C4H5-1p	2.90E+07	2.0	7700.0
1580. C4H6-1+R4CH3=CH4+C4H5-1p	0.00E+00	4.0	8200.0
1581. C4H6-1+B1O=R2OH+C4H5-1p	5.10E+13	0.0	7800.0
1582. C4H6-1+R2OH=>H2O+C4H5-1p	2.70E+06	2.0	-400.0
1583. C4H6-1+O2=>R3OOH+C4H5-1p	1.20E+13	0.0	49000.0
1584. C4H6-1+R3OOH=>H2O2+C4H5-1p	6.00E+11	0.0	17000.0
1585. C4H6-1+B1O=R12CHCOZ+R11C2H5	1.50E+13	0.0	2100.0
1586. C4H6-1+R2OH=CH2COZ+R11C2H5	4.30E+11	0.0	-800.0
1587. C4H6-2=C4H6Z2	3.00E+13	0.0	65000.0
1588. C4H6-2=C4H6-12	3.00E+13	0.0	67000.0
1589. C4H6-2=C4H5-2+R1H	2.00E+14	0.0	87300.0
1590. C4H6-2+R1H=R4CH3+pC3H4	6.50E+12	0.0	1700.0
1591. C4H6-2+R1H=C4H5-2+H2	3.40E+05	2.5	2500.0
1592. C4H6-2+R4CH3=C4H5-2+CH4	4.40E+00	3.5	5700.0
1593. C4H6-2+B1O=B2CO+R10C2H3V+R4CH3	1.50E+13	0.0	2100.0
1594. C4H6-2+B1O=R2OH+C4H5-2	1.20E+11	0.7	7600.0
1595. C4H6-2+R2OH=B2CO+C2H4Z+R4CH3	4.30E+11	0.0	-800.0
1596. C4H6-2+R2OH=C4H5-2+H2O	6.20E+06	2.0	-300.0
1597. C4H6-2+O2=C4H5-2+R3OOH	4.20E+12	0.0	44000.0
1598. C4H6-2+R3OOH=C4H5-2+H2O2	1.90E+04	2.6	13900.0
1599. C4H7-1=C4H7Y	3.34E+09	1.0	39100.0
1600. C4H7-1=C4H7V	3.30E+09	1.0	20700.0
1601. C4H7-1=C2H4Z+R10C2H3V	2.00E+13	0.0	35500.0
1602. C4H7-1+R4CH3=C5H10	2.00E+13	0.0	0.0
1603. C4H7-1+R1H=C4H8Y	1.00E+14	0.0	0.0
1604. C4H7Y+R1H=C4H8Y	2.00E+13	0.0	0.0

1605. C4H7Y+R1H=H2+C4H6Z2	9.00E+12	0.0	0.0
1606. C4H7Y+R1H=H2+C4H6-12	9.00E+12	0.0	0.0
1607. C4H7Y+R3OOH=R2OH+C2H3CHO+R4CH3	1.00E+15	-0.8	0.0
1608. C4H7Y+R4CH3=iC5H10	5.00E+12	0.0	0.0
1609. C4H7V=C4H7Y	1.90E+10	1.0	36300.0
1610. C4H7V=R11C2H5+C2H2	2.00E+13	0.0	33000.0
1611. C4H7-2=C4H7Y	2.90E+10	1.0	37800.0
1612. C4H7-2=R4CH3+pC3H4	2.00E+13	0.0	31500.0
1613. C4H7T=C4H7-1	3.34E+09	1.0	40600.0
1614. C4H7T=C4H7Y	2.00E+13	0.0	47000.0
1615. C4H7T=R4CH3+aC3H4	2.00E+13	0.0	32500.0
1616. C4H8Y+O2=C4H7Y+R3OOH	3.60E+12	0.0	38200.0
1617. C4H8Y+R1H=C4H7Y+H2	5.40E+04	2.5	-1900.0
1618. C4H8Y+R2OH=HCHO+R4CH3+C2H4Z	1.40E+12	0.0	-1000.0
1619. C4H8Y+R2OH=R4CH3+C2H5CHO	1.40E+12	0.0	-1000.0
1620. C4H8Y+R2OH=C4H7Y+H2O	3.00E+06	2.0	-1520.0
1621. C4H8Y+R4CH3=C4H7Y+CH4	1.00E+11	0.0	7300.0
1622. C2H5CHO+R1H=H2+B2CO+R11C2H5	4.00E+13	0.0	4200.0
1623. C2H5CHO+R2OH=H2O+B2CO+R11C2H5	4.00E+12	0.0	500.0
1624. iC4H8+R2OH=iC3H7+HCHO	1.40E+12	0.0	-1040.0
1625. iC4H8+R1H=>iC4H7+H2	3.50E+05	2.5	2510.0
1626. iC4H8+R2OH=>iC4H7+H2O	6.00E+06	2.0	-298.0
1627. iC4H7+R1H=iC4H8	1.00E+14	0.0	0.0
1628. iC4H7+R3OOH=R2OH+HCHO+tC3H5	1.00E+15	-0.8	0.0
1629. C5H7Y+R1H=C5H8	1.00E+14	0.0	0.0
1630. iC5H7Y+R1H=iC5H8	1.00E+14	0.0	0.0
1631. iC5H7Y=aC3H4+R10C2H3V	2.00E+13	0.0	50000.0
1632. C5H8+R1H=C5H7Y+H2	1.70E+05	2.5	2500.0
1633. C5H8+R4CH3=C5H7Y+CH4	2.20E+00	3.5	5670.0
1634. C5H8+R2OH=H2O+C5H7Y	3.00E+06	2.0	-298.0
1635. iC5H8+R1H=iC5H7Y+H2	1.70E+05	2.5	2500.0
1636. iC5H8+R4CH3=iC5H7Y+CH4	2.20E+00	3.5	5670.0
1637. iC5H8+R2OH=H2O+iC5H7Y	3.00E+06	2.0	-298.0
1638. C5H9Y=R1H+C5H8	3.00E+13	0.0	50500.0
1639. C5H9Y+R1H=H2+C5H8	1.80E+13	0.0	0.0
1640. C5H9Y+R1H=C5H10	2.00E+13	0.0	0.0
1641. iC5H9=iC5H9Y	1.70E+09	1.0	38100.0
1642. iC5H9=C3H6Y+R10C2H3V	2.00E+13	0.0	35500.0
1643. iC5H9=iC5H8+R1H	1.60E+13	0.0	34300.0
1644. iC5H9Y=iC5H8+R1H	1.00E+13	0.0	51500.0
1645. iC5H9Y+R1H=H2+iC5H8	1.80E+13	0.0	0.0
1646. iC5H9Y+R1H=iC5H10	2.00E+13	0.0	0.0

1647. iC5H9Y+C3H5Y=iC5H8+C3H6Y	8.40E+10	0.0	-300.0
1648. iC5H9Y+iC5H9Y=iC5H8+iC5H10	8.40E+10	0.0	-300.0
1649. C5H10+R1H=C5H9Y+H2	5.40E+04	2.5	-1900.0
1650. C5H10+R4CH3=C5H9Y+CH4	1.00E+11	0.0	7300.0
1651. C5H10+R2OH=C5H9Y+H2O	3.00E+06	2.0	-1520.0
1652. iC5H10+R1H=iC5H9Y+H2	2.50E+04	2.5	-2800.0
1653. iC5H10+R4CH3=iC5H9Y+CH4	5.00E+10	0.0	5600.0
1654. iC5H10+R2OH=iC5H9Y+H2O	1.30E+06	2.0	-2600.0
1655. C6H4#+R1H=C6H5#	3.00E+17	0.0	36300.0
1656. C6H8#+R1H=H2+C6H7#	1.10E+05	2.5	-1900.0
1657. C6H8#+R2OH=H2O+C6H7#	6.00E+06	2.0	-1520.0
1658. C6H8#=C6H6#+H2	1.28E+28	-4.9	49300.0
1659. C6H10#=C6H9Z#+R1H	5.00E+15	0.0	81400.0
1660. C5H8#=C5H6#+H2	2.20E+13	0.0	60000.0
1661. C5H8-12=C5H8#	1.80E+11	0.0	51826.0
1662. C5H8-12=C5H8	2.20E+14	0.0	67366.0
1663. C5H8-12=C2H4Z+pC3H4	6.60E+12	0.0	58106.0
1664. C5H7#+R1H=C5H8#	1.00E+14	0.0	0.0
1665. C5H7#Y+R1H=C5H8#	1.00E+14	0.0	0.0
1666. C5H7#V+R1H=C5H8#	1.00E+14	0.0	0.0
1667. C5H8#+O2=C5H7#+R3OOH	1.40E+13	0.0	47600.0
1668. C5H8#+O2=C5H7#Y+R3OOH	2.80E+12	0.0	35600.0
1669. C5H8#+O2=C5H7#V+R3OOH	4.00E+12	0.0	55600.0
1670. R1H+C5H8#=C5H9#	1.00E+14	0.0	3260.0
1671. R2OH+C5H8#=>2C2H4Z+R5CHO	2.70E+12	0.0	-1100.0
1672. C5H8#+R1H=C5H7#+H2	9.00E+06	2.0	5000.0
1673. C5H8#+R1H=C5H7#Y+H2	1.08E+05	2.5	-1900.0
1674. C5H8#+R1H=C5H7#V+H2	8.20E+05	2.5	9790.0
1675. C5H8#+R2OH=C5H7#+H2O	2.60E+06	2.0	-770.0
1676. C5H8#+R2OH=C5H7#Y+H2O	6.00E+06	2.0	-1520.0
1677. C5H8#+R2OH=C5H7#V+H2O	2.20E+06	2.0	1450.0
1678. C5H8#+R4CH3=C5H7#+CH4	2.00E+11	0.0	9600.0
1679. C5H8#+R4CH3=C5H7#Y+CH4	2.00E+11	0.0	7300.0
1680. C5H8#+R4CH3=C5H7#V+CH4	1.96E+00	3.5	11700.0
1681. C5H8#+B1O=C5H7#+R2OH	2.60E+13	0.0	5200.0
1682. C5H8#+B1O=C5H7#Y+R2OH	1.70E+11	0.7	3250.0
1683. C5H8#+B1O=C5H7#V+R2OH	1.20E+11	0.7	7630.0
1684. C5H8#+R11C2H5=C5H7#+C2H6	2.00E+11	0.0	11000.0
1685. C5H8#+R11C2H5=C5H7#Y+C2H6	8.80E+00	3.5	4140.0
1686. C5H7#=C5H7#Y	2.30E+11	1.0	44100.0
1687. C5H7#V=C5H7#Y	6.67E+12	0.0	49500.0
1688. C5H7#=C5H7-1s	2.00E+13	0.0	35500.0

1689. C5H7-1s=C2H2+C3H5Y	2.00E+13	0.0	33000.0
1690. C5H7#Y=C5H7Y	1.30E+13	0.0	35900.0
1691. C5H7-1s=C5H7Y	3.40E+13	0.0	34500.0
1692. C5H7-2s=C5H7Y	1.30E+13	0.0	44500.0
1693. C5H7-3t=C5H7Y	5.00E+13	0.0	37000.0
1694. C5H7-4s=C5H7Y	2.00E+13	0.0	47000.0
1695. C5H7-2s=R10C2H3V+aC3H4	2.00E+13	0.0	35500.0
1696. C5H7-3t=R4CH3+C4H4	2.00E+13	0.0	31500.0
1697. C5H7-4s=R10C2H3V+pC3H4	2.00E+13	0.0	31000.0
1698. C5H7#V=C5H7-5p	2.00E+13	0.0	33000.0
1699. C5H7#V=C5H7-12-5p	2.00E+13	0.0	31000.0
1700. C5H7-5p=C2H4Z+C3H3	2.00E+13	0.0	22500.0
1701. C5H7-12-5p=C2H4Z+C3H3	2.00E+13	0.0	35500.0
1702. C5H7#Y=C5H6#+R1H	3.00E+13	0.0	50500.0
1703. C5H9#=C5H9	2.00E+14	0.0	35600.0
1704. C5H9=C3H5Y+C2H4Z	3.30E+13	0.0	22500.0
1705. C5H9=R1H+C5H8	3.00E+13	0.0	38000.0
1706. C5H9=C5H9Y	3.30E+09	1.0	32350.0
1707. C5H9+O2=>C5H8+R3OOH	1.60E+12	0.0	5000.0
1708. C5H7#Y+O2=C5H6#+R3OOH	1.58E+12	0.0	15200.0
1709. C5H7#Y+R3OOH=C2H4Z+CH2CHCO+R2OH	1.00E+13	0.0	0.0
1710. C5H7#Y+R1H=C5H6#+H2	1.80E+13	0.0	0.0
1711. C5H7#Y+R2OH=C5H6#+H2O	6.00E+12	0.0	0.0
1712. C5H7#Y+R4CH3=MCP	1.50E+13	0.0	0.0
1713. MCP+R1H=RMCP1+H2	9.00E+06	2.0	5000.0
1714. MCP+R1H=RMCPY1+H2	5.00E+04	2.5	-1900.0
1715. MCP+R1H=RMCP2+H2	2.90E+07	2.0	7700.0
1716. MCP+R1H=RMCPY2+H2	2.50E+04	2.5	-2790.0
1717. MCP+R2OH=RMCP1+H2O	2.60E+06	2.0	-770.0
1718. MCP+R2OH=RMCPY1+H2O	3.00E+06	2.0	-1520.0
1719. MCP+R2OH=RMCP2+H2O	2.70E+06	2.0	450.0
1720. MCP+R2OH=RMCPY2+H2O	1.30E+06	2.0	-2620.0
1721. RMCP1=C2H2+C4H7Y	2.00E+13	0.0	31000.0
1722. RMCP1=R4CH3+C5H6#	2.00E+13	0.0	31000.0
1723. RMCP2=C2H4Z+nC4H5	2.00E+13	0.0	28700.0
1724. RMCP1+O2=MCPD+R3OOH	2.60E+11	0.0	2500.0
1725. RMCPY1+O2=MCPD+R3OOH	1.58E+12	0.0	15200.0
1726. RMCPY1+R1H=MCP	1.00E+14	0.0	0.0
1727. RMCPY2+R1H=MCP	1.00E+14	0.0	0.0
1728. C5H6#+R4CH3=RMCPY1	9.64E+10	0.0	8000.0
1729. RMCP1+R1H=MCP	1.00E+14	0.0	0.0
1730. C5H5#+R4CH3=MCPD	5.00E+12	0.0	0.0

1731. MCPD+R1H=C5H6#+R4CH3	1.00E+13	0.0	1300.0
1732. MCPD+R1H=RMCP1	2.60E+13	0.0	3200.0
1733. MCPD+R1H=RMCPY1	2.60E+13	0.0	3200.0
1734. MCPD+R1H=RMCPD+H2	2.90E+07	2.0	7700.0
1735. MCPD+R2OH=RMCPD+H2O	2.70E+06	2.0	450.0
1736. MCPD+R1H=RMCPDY+H2	2.50E+04	2.5	-2700.0
1737. MCPD+R2OH=RMCPDY+H2O	1.30E+06	2.0	-2700.0
1738. RMCPDY=RMCPD	3.00E+12	0.0	50400.0
1739. RMCPD=C6H7#	1.40E+13	0.0	17400.0
1740. RMCPDY+R1H=MCPD	1.00E+14	0.0	0.0

NOTE: A units mole-cm-sec-K, E units cal/mole; k = A*(T**b)*exp(-E/RT).

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