DETAILED CHEMICAL KINETIC MODELING OF n-HEPTANE FLAME

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ABSTRACT

DETAILED CHEMICAL KINETIC MODELING OF n-HEPTANE FLAME

To understand the complex combustion characteristics of gasoline, n-heptane is used as one of the two major reference fuels. The emissions resulted from incomplete combustion are one of the main issues caused from usage of high amount of fossil fuels in transportation and energy generation sectors. The main purpose of this study is to model one-dimensional premixed, laminar, burner-stabilized fuel-rich n-heptane flame to understand its combustion characteristics in mainly fuel-rich conditions. Detailed chemical kinetic modeling technique was used to get high amount of information about the ignition characteristics of n-heptane and formation nature of emissions. A detailed chemical kinetic mechanism was generated by combining several mechanisms from the literature that related with possible products of fuel-rich n-heptane combustion. The detailed mechanism consists of 4185 reactions and 893 species. Validations of the model were done with various experimental data available in the literature such as premixed laminar flames and jet stirred reactors. After generating the kinetic model, detailed investigation of the n-heptane flame was done by using rate of production, reaction sensitivity and reaction pathway analyses. One of the attributes of fuel-rich flames, Polycyclic aromatic hydrocarbon (PAH) formation kinetics were also investigated. Acetylene (C_2H_2), propargyl radical (C_3H_3), and vinylacetylene (C_4H_4) were found as the main precursors of the first aromatic ring and PAH formation as a result of pathway and rate of production analyses. The generated model was able to predict most of the major, minor and trace components that formed in the flame that modeled. A reduced model was also generated by using directed relation graph with error propagation (DRGEP) mechanism reduction technique on the detailed mechanism. The reduced mechanism consists of 1879 reactions and 359 species. The species mole fraction predictions of detailed and reduced mechanism were very close to each other. Most of the species formed in the flame were predicted by the reduced mechanism with less computational afford than detailed mechanism.

ÖZET

DETAYLI KİMYASAL KİNETİK MODELLEME ILE n-HEPTAN YANMASININ MODELLENMESİ

Benzinin karmaşık yanma özelliklerini anlamak için kullanılan iki ana referans yakıttan birisi n-heptandır. Ulaşım ve enerji üretimi sektörlerinde yüksek miktarda fosil yakıt kullanımı nedeniyle ortaya çıkan temel sorunlardan birisi eksik yanma sonucu açığa çıkan emisyonlardır. Bu çalışmanın temel amacı, yakıt açısından zengin koşullarda n-heptanın yanma özelliklerini anlayabilmektir. Bu sebeple tek boyutlu önceden karıştırılmış, laminar, yakıt bakımından zengin n-heptan alevi detaylı kimyasal kinetik modelleme (DKKM) tekniği kullanılarak modellenmiştir. DKKM tekniği sayesinde n-heptanın tutuşma özellikleri ve emisyonların oluşum özellikleri kapsamlı bir sekilde incelenebilmiştir. Literatürden çeşitli mekanizmaların birleştirilmesiyle detaylı bir kimyasal kinetik mekanizma oluşturulmuştur. Detaylı mekanizma 4185 reaksiyon ve 893 türden oluşmaktadır. Modelin doğrulanması, literatürden elde edilen önceden karıştırılmış laminar alevler ve jetle karıştırılan reaktörler gibi çeşitli deneysel verilerle yapılmıştır. Kinetik model oluşturulduktan sonra, n-heptan alevinin ayrıntılı araştırması, üretim hızı, reaksiyon duyarlılığı ve reaksiyon yolu analizleri kullanılarak yapılmıştır. Yakıt açısından zengin alevlerin özelliklerinden biri olan polisiklik aromatic hidrokarbon (PAH) oluşumunun kinetiği de araştırılmıştır. Üretim hızı analalizleri sonucu asetilen (C_2H_2), propargil radikali (C_3H_3) ve vinilasetilen (C_4H_4) ilk aromatik halkanın ve PAH oluşumunun ana öncüleri olarak bulunmuştur. Modellenen alevde oluşan birincil (major), ikincil (minor) ve eser türlerin çoğu geliştirilen mekanizma ile tahmin edilmiştir. Detaylı modelde mekanizma indirgeme tekniği kullanılarak oluşturulan iskelet bir mekanizma da geliştirilmiştir. İndirgenmiş mekanizma 1879 reaksiyon ve 359 türden oluşmaktadır. İndirgenmiş mekanizma, alevde oluşan bileşiklerin çoğunu daha az hesaplama gücü kullanarak tahmin edebilmeyi başarmıştır.

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CHAPTER 1

INTRODUCTION

As an applied science combustion has a variety of application areas such as power generation, transportation, and industrial manufacturing operations. Most of the energy that is being utilized comes from numerous combustion-related sources. That is why environmental considerations, efficiency and safety concerns must be examined together in practical combustion studies.

Rise on the worldwide energy demand resulted in an increase in the amount of combustion-related power generations process. In the earlier years of the industrial era providing the necessary amount of fuel in a cost-effective way was the main problem. However, emission of hazardous side-products from combustion applications became the top issue in recent years. The main sources of precarious components of combustion operations are internal combustion engines, jet engines, rocket engines, thermal power plants and some manufacturing processes. Reducing the emissions from the combustion operations are still discussed in science circle. The environmental regulations lead up to new trends such as alternative fuels, low emission technologies and higher efficiency requirements in terms of energy generated per fuel consumed.

The major emissions of combustion processes can be considered as carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxides (NO_x), unburned/partially burned hydrocarbons (UHC), polycyclic aromatic hydrocarbons (PAH), sulfur oxides (SO_x), and particulates (soot, fly ash, aerosols). The products of the combustion depend on the fuel type and the operating conditions such as temperature, pressure and equivalence ratio. However, the chemistry behind the oxidation of the fuel is the main factor that determines the products, side-products, and the temperature-pressure behavior of the combustion. Therefore, the chemical kinetics of the combustion needs to be investigated deeper to enhance the operations in a productive manner. Effects of the parameters on the formation of pollutants can be examined using chemical kinetics. Gasoline is one of the most common fuels utilized in land transportation. Figure 1.1 shows the world energy usage at transportation by sources. As seen from Figure 1.1, the projections state that gasoline will be remained to be the main fuel of transportation on the following 30 years.

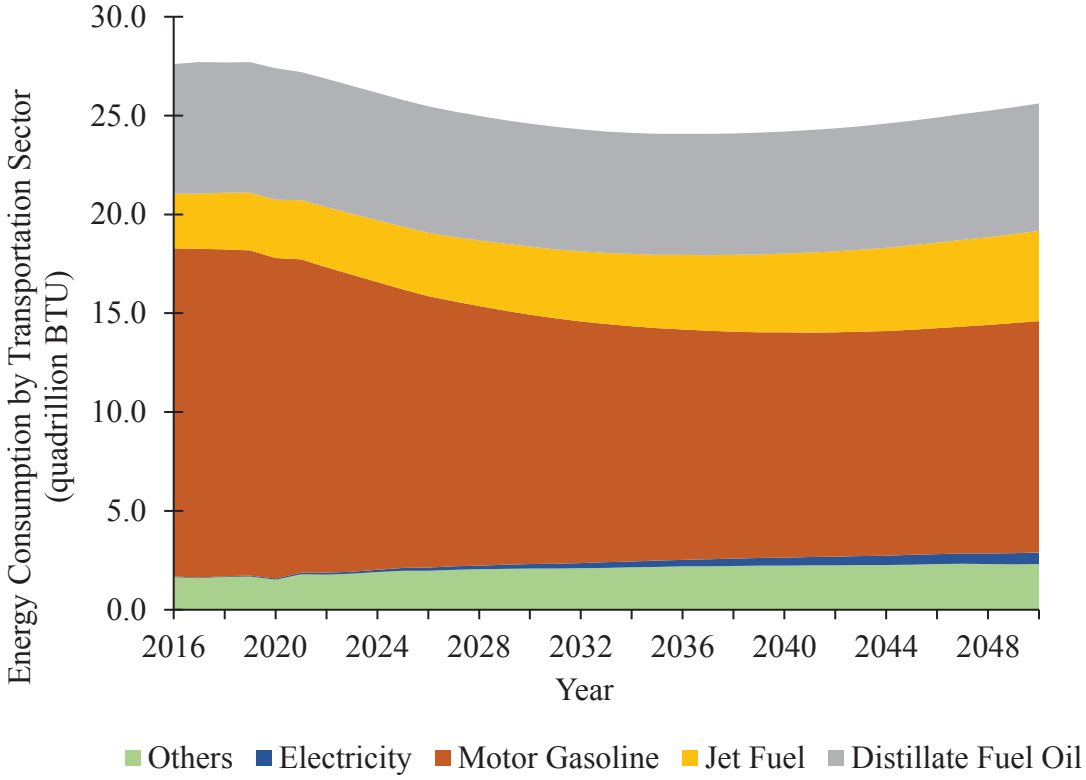

Figure 1.1. World transportation sector energy consumption by energy source (AEO 2018)

Gasoline, which contains hundreds of chemical species, mostly 4 to 12 carbons per molecule, mainly contains saturated-hydrocarbons. This complex nature of the gasoline forces scientists to come up with a classification method to show auto-ignition characteristic. The auto-ignition behavior is one of the most important properties of a fuel for the spark ignition engines because it is related with engine knock. To measure the auto-ignition behavior of gasoline, iso-octane (i-C_8H_{18}) and n-heptane (C_7H_{16}) are used as reference components for the octane number (ON) determination. By definition, iso-octane has 100 ON (low knocking tendency) and n-heptane has 0 ON (high knocking tendency).

n-Heptane (C_7H_{16}) is considered as gasoline representative fuel for combustion modeling along with toluene (C_7H_9) and iso-octane (i-C_8H_{18}). The modeling of n-heptane combustion gives excellent information about the emission control and performance of gasoline engines. Auto-ignition behavior of the gasoline can also be understood in molecular-level by detailed chemical kinetic modeling.

Polycyclic aromatic hydrocarbons (PAHs) consist of two or more aromatic rings that bonded with linear, angular or cluster form in their structure. Most of the polycyclic

aromatic hydrocarbons are toxic and carcinogenic compounds (Larsen 2013). The high solubility of PAHs on lipids result in accumulation on the body fat. Exposure to PAH can cause to lung and skin cancer. The sources of PAH emission can be classified as stationary, mobile and natural sources. Natural sources can be listed as forest fires and volcano eruptions. The stationary sources of PAH emission are industrial and household sources and the mobile sources are automobiles that utilize diesel or gasoline. The main reason behind PAH formation is the incomplete combustion of the fuel. PAHs can be formed from combination of simpler aromatic rings such as benzene (C_6H_6) or they can also be formed as an aromatic compound from non-aromatic species. Heavier PAHs such as coronene ($C_{24}H_{10}$) are considered as precursors of the soot particles at flames by planar growth and coagulation (Frenklach and Wang 1991) .

Figure 1.2 shows the gas phase PAH emissions for a gasoline vehicle with commercial unleaded gasoline fuel (Hall et al. 1998). The testing cycle for the study was the US Federal Test Procedure (FTP-75). Phenanthrene had the highest emission with around 90 (µg/km) for the engine used in the test. The value for total gas-phase PAH emission corresponds to $0.066 \frac{g}{Year \times Car}$ when average car usage is taken as 20,000 km/year in the USA.

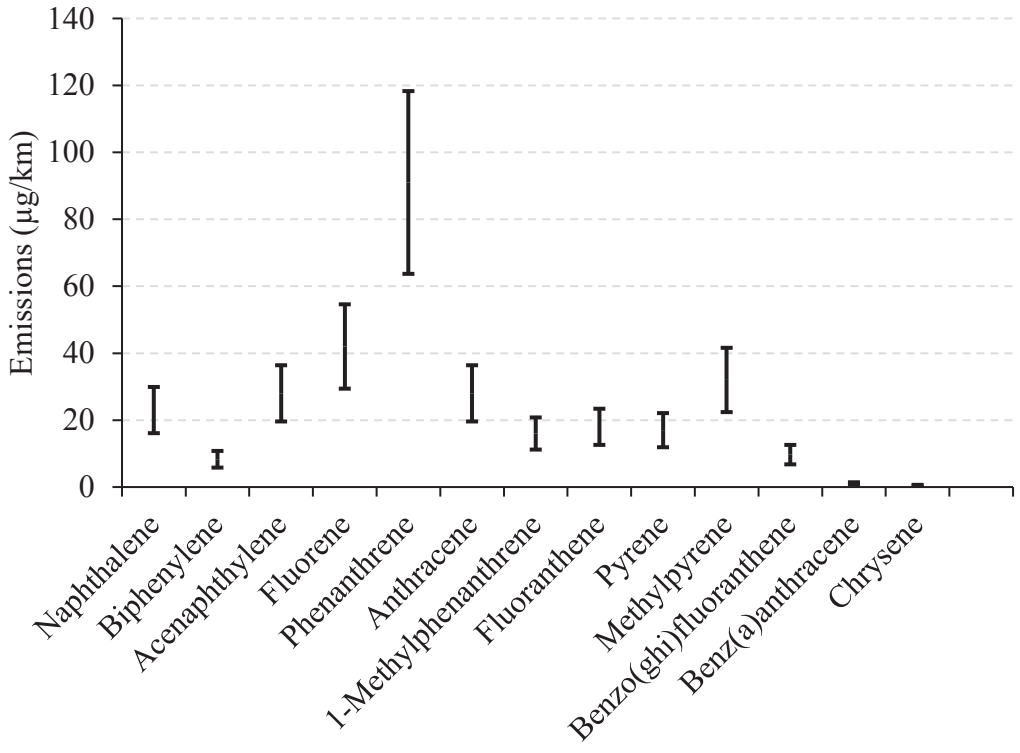

Figure 1.2. Gaseous PAH emissions for a gasoline vehicle

Experiments on mice and rats were shown that even in ppm level concentrations, most of the PAHs have similar health effects with benzo[a]pyrene which is a known carcinogen, mutagen and toxic substance. (Schneider et al. 2002).

The computational solutions have become more extensive in most of the engineering areas in last decades. However, to apply a computational solver in an engineering field, a good level of knowledge in the research area is required. Chemical engineering knowledge in molecular level is fundamental for modeling combustion phenomena. Basically, modeling is the mathematical description of a system with equations that represent the physical behavior of the system of interest. The package of elementary reactions, thermodynamic properties and molecular transport data which is required to model combustion in molecular level is called as the detailed chemical kinetic mechanism (DCKM). The kinetic parameters of the elementary reactions are the main components of the detailed chemical kinetic mechanism. Combustion reactions are very fast thus cause almost instantaneous temperature and pressure shifts in the system. Thermodynamics determine the limits so that it is also required to be included. In most cases, the molecular transport properties of the species are also essential. Systems such as diffusion flames and flow reactors, mass transfer can be the limiting factor rather than chemical kinetics so that transport properties are needed to be considered. The formation and consumption of the species in the detailed kinetic mechanism put into design equations and solved together with the thermodynamic properties. The design equations depend on the system of interest, they can be either differential or algebraic equations. The resulting parameters of the simulations, such as species concentrations, temperature, pressure, and ignition delay times required to be verified by comparing with experimental studies, that procedure is called mechanism validation.

In this study, the objective is to model fuel-rich, atmospheric pressure n-heptane flame by using DCKM technique. Chemkin-Pro® (Kee et al. 1996) software were used to model the systems. The main reason for selecting fuel-rich flame was to set oxidizer as the limiting reactant which results in incomplete combustion. By this way the emissions of the incomplete combustion could be seen. Some hydrocarbons that formed in such condition can't be oxidized properly and they are referred as partially burned hydrocarbons. The formation kinetics of partially burned hydrocarbons, benzene and, polycyclic aromatic hydrocarbons, in fuel-rich n-heptane flame was investigated by using detailed chemical kinetic modeling techniques. The parameters that affect the formation kinetics of various PAHs up to 4 ring structures such as pyrene ($C_{16}H_{10}$), phenanthrene

($C_{14}H_{10}$) and their precursors were discussed. The rate of production/consumption analyses and pathway analysis were done to understand n-heptane oxidation. Additionally, a reduced kinetic mechanism for n-heptane oxidation was generated to simulate the n-heptane combustion with less computational effort.

CHAPTER 2

LITERATURE SURVEY

2.1. General Features of Hydrocarbon Combustion

Parameters that designate the products and by-products of the combustion operations can be listed as temperature, pressure and the equivalence ratio. The essence behind those effects are the reaction rates of the elementary reactions.

Equivalence ratio (ϕ) is used to define the oxidizer and fuel mixture. If equivalence ratio is greater than 1 the amount of oxidizer is not enough to oxidize the fuel completely which corresponds to fuel-rich conditions. If equivalence ratio is less than 1 the oxidizer amount is more than required for complete combustion of fuel which corresponds to fuel-lean conditions. For stoichiometric fuel-oxidizer mixtures, equivalence ratio is 1. Equivalence ratio can be calculated by the following equation.

$$\phi = \frac{\left(\frac{\text{Oxidizer}}{\text{Fuel}}\right)_{\text{Stoichiometric}}}{\left(\frac{\text{Oxidizer}}{\text{Fuel}}\right)_{\text{Actual}}} \tag{2.1}$$

The combustion mechanisms of the saturated hydrocarbons are very similar with an exception of methane (CH_4). The exception of methane is caused by higher bonding energies between carbon and hydrogen atoms due to the unique tetra hexagonal structure.

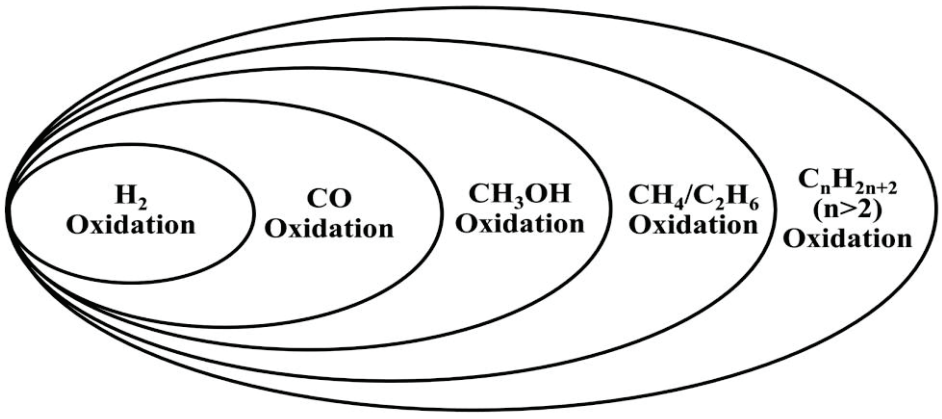

Figure 2.1. The hierarchy of the alkane combustion (Warnatz, Maas, and Dibble 2006)

As seen from Figure 2.1 the oxidation mechanism of alkanes with the higher number of carbons involves at least C_1, C_2, H_2, and CO oxidation mechanisms.

The temperature of the system has a significant effect on hydrocarbon oxidation. The progress of combustion highly depends on free radical species such as (H, O, OH, HO_2, CH_3) which are unstable and react very fast. Since there are no radicals at early stages, the main step to increase the radical pool is the direct collision with fuel radical (R) and O_2 (reaction 1). The main pathways that generate the radical pool depend on the temperature. At low temperatures, up to 700 K, the chain branching reaction (reaction 2) increases the radical concentration exponentially.

$$R + O_2 \leftrightarrow ROO \quad (R1)$$

$$RO_2 \leftrightarrow R'OOH \leftrightarrow R'O + OH \quad (R2)$$

Around 650 K to 700 K ROO decomposition by the reverse reaction 1 become faster than the forward reaction which causes slower chain branching and slower overall reaction, that phenomena are called negative temperature coefficient (NTC).

At intermediate temperatures, the main pathway to generate radicals relies on HO_2 and H_2O_2 species, basically, HO_2 and H_2O_2 take the roles of ROO and R′OOH respectively (reaction 3, 4 and 5). The chain branching reaction (reaction 5) increase the radical pool instantaneously.

$$H + O_2 + M \leftrightarrow HO_2 + M \quad (R3)$$

$$RH + HO_2 \leftrightarrow R + H_2O_2 \quad (R4)$$

$$H_2O_2 + M \leftrightarrow OH + OH + M \quad (R5)$$

At high temperatures hydrogen radicals are not rate limiting because of faster H abstraction rate from fuel and smaller alkanes, so that the main path that produces high amounts of radical is reaction 6;

$$H + O_2 \leftrightarrow O + OH \quad (R6)$$

Additionally, at high temperatures which corresponds to the main reaction zone for flames, reaction 7 is the key reaction that releases heat and ensures the continuity of chain reactions.

$$CO + OH \leftrightarrow CO_2 + H \quad (R7)$$

2.2. n-Heptane Oxidation

Since n-heptane is considered as primary reference fuel for gasoline, there have been many studies about its detailed chemical kinetic mechanism. Product species analyses on flames are the major types of experimental and modeling studies. Several reactor types such as jet-stirred reactor, plug flow reactor, and variable pressure reactor are the main systems to develop and validate the DCKM with species concentration predictions in the literature. Additionally, in the literature ignition delay time measurements are usually done with rapid compression machines. The ignition delay time predictions are another key parameter for mechanism validation.

A semi-detailed mechanism for n-heptane and iso-octane mixtures with 41 species and 116 reactions were generated based on the numbers of primary, secondary or tertiary C-H bonds that formed from the initial fuel molecules (Griffiths et al. 1994). Abstraction, branching, and propagation reactions were involved in the mechanism, by comparing the experimental data taken from shock tube and rapid compression machine experiments. The kinetic mechanism was validated for especially at low temperatures ($650<T<850$) by ignition delay time predictions.

A semi-detailed kinetic mechanism for primary reference fuel mixture (n-heptane and iso-octane) were generated with simplified propagation schemes and detailed kinetics for smaller components (Callahan et al. 1996). Comparisons with the kinetic model were done with ignition delay time data from a rapid compression machine. Product species analyses (H_2O, CO, CO_2 and O_2) and heat release were done with variable pressure reactor experiments. As a result, the model was showed good performance at the temperature range of 550 to 1250 K, the pressure range of 0.02 to 2 MPa and at the equivalence ratio of 1.

A semi-empirical chemical kinetic mechanism for n-heptane oxidation and pyrolysis that involves about 270 reactions and 40 species were designated (Held, Marchese, and Dryer 1997). Premixed flame speed calculations of the model was compared with several experimental data from literature in the equivalence ratio range of 0.7 to 1.5. Additionally, shock tube experimental data were used to validate the model in terms of ignition delay time.

A detailed chemical kinetic mechanism that consists of 990 species and 4060 reactions for primary reference fuel (n-heptane) were generated (Curran et al. 1998). The

mechanism was validated by the experimental data that were done similar to engine conditions, in the equivalence ratio range from 0.3 to 1.5 and high pressures up to 42 atm and temperature range of 550 to 1700 K. High-pressure flow reactor was used to analyze species concentrations such as H_2O, CO, CO_2, and O_2. Shock tubes were used to validate the model in terms of ignition delay time. Good agreement between experimental data and model predictions were achieved.

An experimental study of laminar premixed O_2/n-heptane/N_2 flame was carried out with the equivalence ratio of 1.9. (Bakali, Delfau, and Vovelle 1998) Species concentration profiles for intermediates, major and minor products were measured over the flame by using microprobe and online GC/MS system. Soot formation was also examined but not measured quantitively.

Another experimental study that focus on the formation of polycyclic aromatic hydrocarbons (PAH) in fuel-rich n-heptane flames was done by Inal and Senkan, (2002). Two atmospheric pressure, premixed, laminar n-heptane flames with equivalence ratios of 1.97 and 2.1 were studied. The species mole fraction profiles up to four ring PAHs with respect to burner height were measured by the online GC/MS and GC/TCD analyses. The soot formation on the flames were also measured by using light scattering technique.

High-temperature oxidation and pyrolysis mechanism of PRF mixtures that involves 107 species and 723 reactions was established (Chaos et al. 2007). Premixed flame speed and ignition delay time data were used to validate the mechanism. The model showed good performance at temperatures greater than 950 K, pressures less than 15 bar and equivalence ratio less than 2.5.

A detailed chemical kinetic mechanism that explains the formation of polycyclic aromatic hydrocarbons up to four ring structures and soot from several fuels (n-heptane, iso-octane, and decane) were studied (Marchal et al. 2009). The mechanism consists of 101 species and 1001 reactions by taking into account forward and reverse reactions separately. The mechanism involves PAH formation kinetics for species up to pyrene (A_4) and validated by comparing premixed laminar flames of n-heptane and iso-octane. However, the validations were done for a n-heptane flame that did not include PAH species. Additionally, several jet-stirred reactor experimental data of species concentrations up to benzene and its precursors were also used for validations, in the temperature range of 750 to1150 K and pressure of 1 MPa.

A gasoline surrogate (n-heptane, iso-octane, and toluene) detailed chemical kinetic mechanism for a wide range of engine conditions was proposed (Mehl et al. 2011).

The merged mechanism consists of ~8000 reactions and ~1550 species. Validations were done with numerous experimental data for both pure fuels and various fuel blends such as toluene/n-heptane, iso-octane/1-hexene. The results of the validations on JSR and shock-tubes shown that the model was highly successful for the ignition essentials in equivalence ratio of 1 and the pressure and temperature ranges of 3 to 50 atm and 650 to 1200 K, respectively.

A detailed kinetic mechanism of n-heptane that consists of 1400 reactions and 350 species for the growth pathways of large PAH was developed (Raj et al. 2012). Density functional theory (DFT) and transition state theory (TST) were used to determine reaction kinetics for some PAH reactions. However, the mechanism did not consider the formation of linear PAH such as anthracene. Experimental data of premixed laminar n-heptane, iso-octane, benzene and ethylene flames at atmospheric pressures were used to validate the mechanism by species concentration profiles. For benzene formation, CH_3 and C_5H_5 reaction pathways were also included in the mechanism. Alternative formation pathways for naphthalene ($C_{10}H_8$), phenanthrene ($C_{14}H_{10}$), pyrene ($C_{16}H_{10}$) were also involved in the mechanism. Moreover, the formation pathways of several larger aromatic structures up to coronene were also added from various kinetic data in the literature. There was a good agreement between the experimental data and model predictions.

A reduced chemical kinetic mechanism for gasoline reference fuel which consists of toluene, iso-octane and n-heptane were proposed (Wang et al. 2015). The mechanism consists of 109 species and 543 reactions. Simplified PAH formation kinetics were also involved in the mechanism. Shock tube experimental data and homogenous charge compression engine data were used to validate the mechanism in terms of ignition delay time. Product species that include polycyclic aromatic hydrocarbons, and flame speed analysis were done with experimental data from premixed flames. Reaction sensitivity analysis for PAH formation was also performed and it showed that for benzene formation, the most effective reactions were between $C_4 + C_2 \rightarrow$ Benzene and $C_3 + C_4 \rightarrow$ Benzene for a non-aromatic fuel. For PAH formation, most effective reactions were determined as $C_5 + C_5 \rightarrow$ Naphthalene and the well-known hydrogen abstraction acetylene addition (HACA) mechanism. The model showed fine performance on the experimental data that examined. Just three main PAH were involved in the mechanism (i.e. naphthalene, phenanthrene and, pyrene).

A low pressure (40 mbar) premixed n-heptane flame with the equivalence ratio of 1.69 was carried out (Seidel et al. 2015). The mole fractions profiles for intermediates,

major products, and minor products were inspected by using molecular beam mass spectrometry (MBMS). The concentration profiles of ~80 species up to naphthalene ($C_{10}H_8$) were determined. A detailed chemical kinetic mechanism with 349 species and 3686 reactions was also generated by using the experimental data of the study. Model predictions were shown acceptable performance on estimating species concentration, flame speed and ignition delay time predictions at the pressures ranges of 1 bar to 40 bar and at temperature ranges of 500 K to 2000 K.

A semi-detailed chemical mechanism that clarifies the formation of PAH species from toluene reference fuel was proposed (An et al. 2015) The mechanism consist of 219 species and 1229 reactions. The validations were done by both ignition delay time with a temperature range of 750 to 1280 K, pressure range of 15 to 60 bar, and equivalence ratios from 0.5 to 2.0. Laminar flame speeds were also used to validate the mechanism with various pressures. Moreover, comparisons between species concentration data on premixed laminar flames from various studies were also used to validate the mechanism. Rate of production /consumption analyses were done to examine the most effective reactions in the product concentration of benzene. It was observed that reaction rates of benzene formation were highly dependent on temperature. For relatively low temperature range (700 K to 950 K) n-C_4H_5 +C_2H_2 ←→ A_1 + H (A_1 refers to benzene) was determined as the most important reaction. For moderate temperatures, AC_3H_4 + C_3H_3 ←→ A_1 + H reaction was found as an important reaction for first aromatic ring formation (800 K to 1400 K). A_1- + CH_4 ←→ A_1 + CH_3, (A_1- refers to phenyl) $C_6H_5CH_3$ + H ←→ A_1 + CH_3 ($C_6H_5CH_3$ refers to toluene) and C_3H_3 + C_3H_3 ←→ A_1 (C_3H_3 refers to propargyl) were considered as most the important reactions for high temperatures benzene formation (1200 K to 1530 K). Better overall performance was achieved from this model than the model of Raj et al. (2012).

Park et al. (2017) developed a detailed chemical kinetic mechanism that describes the formation of PAH species up to coronene from the gasoline reference fuels (iso-octane, n-heptane, toluene). The overall mechanism consists of 2021 species and 8688 reactions. Additionally, a high-temperature sub-mechanism that consist 574 species and 3379 reactions was also proposed for premixed laminar flames and counter-flow diffusional flames. Soot formation mechanisms from pyrene (A_4) and higher PAH species were also studied. To understand the effect of non-premixing flames an experimental set-up that involves counter flow diffusion flame was conducted. Laser-induced fluorescence (LIF) technique was used to analyze the relative PAH concentration. Laser induced

incandescence (LII) was used to determine soot volume fractions. Validations of the mechanism were done by ignition delay times in shock tube data, laminar burning velocities, and the species concentration profiles of premixed and partially premixed laminar flame experimental data. The model showed good overall performance for ignition delay time simulations. However, the flame speed simulations at atmospheric pressure for fuel-rich region was slightly underestimated the flame speeds.

As appeared from literature survey on n-heptane oxidation, because of its importance as a reference fuel, there are many of studies on combustion characteristics of n-heptane and its mixtures both experimental and modeling wises. However, there are limited number of studies that worked with the guide of experimental data from fuel-rich one-dimensional premixed laminar n-heptane flame. As a characteristic of a fuel-rich hydrocarbon flame, emissions such as aromatic rings and polycyclic aromatic hydrocarbons appears on the flame. The next section is about the proposed formation pathways for the first aromatic ring.

2.3. Formation of First Aromatic Ring

There have been numerous studies on the formation mechanism of the first aromatic ring since it is the main source of polycyclic aromatic hydrocarbons (PAH) formation during combustion. Benzene is considered as one of the first aromatic ring formed in flames. Acetylene (C_2H_2) was the one of the most recognized compounds that causes formation of benzene (Palmer and Cullis 1965). 1-3 Butadiene (C_4H_6) flames have shown that 1-3 butadienyl radical (C_4H_5) was an another precursor for benzene formation by the following mechanism (Cole et al. 1984).

$$1\text{-}3\ C_4H_5 + C_2H_2 \rightarrow C_6H_7 \qquad \text{(R8)}$$

$$C_6H_7 \rightarrow \text{c-}C_6H_7 \text{ (ring closure)} \qquad \text{(R9)}$$

$$\text{c-}C_6H_7 \rightarrow C_6H_6 + H \text{ (hydrogen loss)} \qquad \text{(R10)}$$

Following studies were suggested that more pathways are necessary to explain benzene formation by considering thermodynamic and structural examinations. C_3H_3 radical was suggested to be a precursor of the first aromatic ring by the following mechanism (Melius, Miller, and Evleth 1992).

$$C_3H_3 + C_3H_3 \leftrightarrow C_6H_5 + H \qquad \text{(R11)}$$

$$C_3H_3 + C_3H_2 \leftrightarrow C_6H_5 \quad \text{(R12)}$$

Cyclopentadiene (c-C_5H_6) was also granted to play a role in the formation of benzene and following mechanism (Dente, Ranzi, and Goossens 1979).

$$C_2H_4 + C_5H_6 \rightarrow C_6H_6 + H + CH_3 \quad \text{(R13)}$$

Other potential precursors for benzene formation were suggested as C_5H_5 (Moskaleva, Mebel, and Lin 1996) propyne (C_3H_4) (Wu and Kern 1987) and ethylene (C_2H_4) (Dente, Ranzi, and Goossens 1979).

It was also suggested as recombination of but-1-ene-3-yne (diacetylene, C_4H_4) radicals result with the formation of phenylacetylene (C_8H_6) as an alternative first aromatic ring in combustion (Lin et al. 2016).

After the formation of first aromatic ring various growth pathways resulted in PAH formation. Pathways that were suggested for PAH formation is reviewed in the next section.

2.4. Formation of Polycyclic Aromatic Hydrocarbons (PAH)

Hydrogen abstraction acetylene addition (HACA) was the first discovered pathway that results in the formation of polycyclic aromatics (Frenklach and Wang 1991). That mechanism relied on the addition of acetylene to benzene radicals to grow their molecule and after the necessary amount of carbon is achieved two-membered and more aromatic species is generated by rotation of the tip of the linear side.

$$A_i + H \leftrightarrow A_i\text{-} + H_2 \quad \text{(R14)}$$

$$A_i\text{-} + C_2H_2 \leftrightarrow A_iC_2H_2 \quad \text{(R15)}$$

$$A_iC_2H_2 + C_2H_2 \rightarrow A_{i+1} + H \quad \text{(R16)}$$

where A_i is the aromatic species with i number of aromatic rings.

Diacetylene addition to aromatic radical and fusion of aromatic radical with an aromatic ring also considered as growth mechanism of polycyclic aromatics (Appel, Bockhorn, and Frenklach 2000).

$$A_i\text{-} + C_4H_4 \leftrightarrow AiC_4H_4 \rightarrow A_{i+1} \quad \text{(R17)}$$

$$A_1\text{-} + A_1 \rightarrow P_2 \quad \text{(R18)}$$

where P_2 is biphenyl.

For the formation of higher angular polycyclic aromatic hydrocarbons such as phenanthrene (A_3) lesser amount of carbon addition is sufficient (Frenklach 2002).

$A_1\text{-} + A_1C_2H \rightarrow A_3$ (R19)

$A_2\text{-} + C_2H_2 \rightarrow A_3 + H$ (R20)

Cyclopentadienyl radical C_5H_5 was also suggested to be taking a role in the formation of two-membered polycyclic aromatic hydrocarbon, naphthalene ($C_{10}H_8$) (Ikeda et al. 2000).

$C_5H_5 + C_5H_5 \rightarrow A_2 + H + H$ (R21)

Recent suggestions for PAH growth mechanism hydrogen abstraction methyl addition (HAMA) was considered to be taking a role in the growth of smaller aromatic hydrocarbon species such as indene (C_9H_8) (Hansen et al. 2017).

From the literature survey chapter, it is understood that n-heptane is one of the major reference components for internal combustion engine fuel standards. To understand the combustion characteristics of n-heptane mainly in fuel-rich conditions, detailed chemical kinetic modeling technique will be exerted on the premixed laminar n-heptane flame experimental study of Inal and Senkan (2002). The experimental study (Inal and Senkan 2002) will be simulated to analyze the dominant reactions on formation of emissions (aromatic hydrocarbons, partially burned hydrocarbons, etc.). The decomposition characteristics of n-heptane will also be investigated. Next chapter is mainly about the modeling technique that was used in this study. Additionally, information about the study of Inal and Senkan (2002) will be given in next chapter, the experimental data from that study was used for model generation and analysis.

CHAPTER 3

METHODS

3.1. Theory of Chemical Kinetic Modeling

When we go down into the details of the combustion the elementary reactions are the keystones. The elementary reactions can be simple solely but when the amount of reactions increases the numerical solutions become harder. The improvements of computational technology which include increase in computer processing capacity and the software developments make the detailed chemical kinetic modeling possible. The chemical kinetic models help us to find out production/consumption of desired/undesired/intermediate species. It also helps us to understand the effective reactions for several phenomena such as ignition delay and heat release. Moreover, it is also capable of computing the effect of the operating conditions which assists us to simulate the reactions in almost limitless conditions.

Increasing trend of usage of detailed chemical kinetic modeling also enhance the available databases for the gas phase kinetics, thermodynamic properties, and transport properties. Additionally, developments in both theoretical approaches such as quantum mechanical computations of the reaction rate constants reduced the relative error in kinetic modeling. Moreover, with the improvements in experimental characterization techniques, the relative error in reference data for model validations was also minimized.

Despite the number of alternative software available for detailed chemical kinetic modeling, one of the most convenient application in this purpose is CHEMKIN® (Kee et al. 1996). The NASA input data format (McBride, Gordon, and Reno 1993) that includes kinetic rate parameters, thermodynamic properties and transport properties is utilized in CHEMKIN. The conservation equations including continuity of mass, momentum, and energy are required to be solved to model reactive flow system. Variations of species concentrations due to chemical reactions make the energy equations difficult to solve. For the combustion systems, kinetic terms are very effective on time and space so that the complex equations must be handled. The equations for flame modeling will be described in next sections in this chapter.

CHEMKIN utilizes three databases which are the chemical kinetic database, thermodynamic database and, transport properties database to solve design equations of the various reactor and flame models.

3.2. Chemical Rate Expressions

High number of elementary reactions exist in detailed chemical kinetic mechanisms to explain heat release, emissions, and ignition phenomena. So that the rate expressions of each elementary reaction must be present in the database. The kinetic database includes each species, elements and elementary reactions with rate parameters.

To describe temperature and bonding energy dependence of elementary reactions, modified Arrhenius expression is used.

$$k_{fi}=A_i T^{B_i} e^{\frac{Ei}{RT}} \tag{3.1}$$

where k_{fi} is the forward rate constant, A_i is the pre-exponent collision frequency factor, B_i is the temperature exponent, E_i is the activation energy, T is the temperature, and R is the universal gas constant.

For small temperature ranges temperature exponent (B_i) is generally zero. However, in large temperature ranges non-Arrhenius behavior can be achieved for combustion reactions so B_i need to be described. Some reactions (i.e. termolecular reactions) require a third body (M) to overcome the energy barrier. The third body is the total concentration, however, some species act as collision partner more effectively than others so that effective third body need to be specified.

The reverse rate constants are usually calculated by using equilibrium constants,

$$k_{ri} = \frac{k_{fi}}{K_{ci}} \tag{3.2}$$

where k_{ri} is the reverse rate constant and K_{ci} is the equilibrium constant.

The equilibrium constant is generally calculated from thermodynamic properties to decrease uncertainty, which will be described in next section.

Rate of progress variable is used to declare that the rate-of-progress of a reaction. For a system that has chemical reactions that consists K species, the elementary reactions are described as;

$$\sum_{k=1}^{K} v'_{ki}\, X_k \leftrightarrow \sum_{k=1}^{K} v''_{ki}\, X_k \tag{3.3}$$

where v_{ki} is the stoichiometric coefficient, X_k is the mole fractions for the k^{th} species superscript $'$ and $''$shows the forward and reverse reactions respectively.

$$q_i = k_{fi} \prod_{k=1}^{K} [X_k]^{v'_{ki}} - k_{fi} \prod_{k=1}^{K} [X_k]^{v''_{ki}} \tag{3.4}$$

where q_i is the rate of progress variable and $[X_k]$ is the molar concentration. The production rate of k^{th} species ($\dot{w}_{ki}$) can be written as the summation of progress variables of all reactions.

$$\dot{w}_{ki} = \sum_{i=1}^{K} v_{ki} q_i \tag{3.5}$$

$$v_{ki} = v'_{ki} - v''_{ki} \tag{3.6}$$

Basically, the kinetic database consists of all species and their elementary reactions, modified Arrhenius parameters and pressure dependence along with them. Forward rate constants of the elementary reactions are calculated by using kinetic database. The reverse rate constants are generally calculated by using equilibrium rate constants. However, it is also possible to write reverse rate constants on the kinetic database.

```
 Reactions                                        Ai          Bi         Ei
H+O2<=>O+OH                                    1.040E+14     .000   15286.00
2H+M<=>H2+M                                    1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
2H+H2<=>2H2                                    9.000E+16    -.600        .00
```

Figure 3.1. Input data format for chemical kinetic database

Figure 3.1 shows the input parameters for chemical kinetic properties, (chemical reactions, pre-exponent factor, temperature exponent and activation energy for each reaction). Additionally, third body efficiencies for termolecular reactions are also required as at the last reaction in Figure 3.1.

3.3. Thermodynamic Properties

Thermodynamic properties of species are also required to perform detailed chemical kinetic modeling. Thermodynamics database is used to define the thermodynamic properties of all species using seven coefficient polynomial fittings for temperature dependence. NASA equilibrium code (Gordon and McBride 1971) is used to define standard state properties of entropy (S_k^o), enthalpy (H_k^o), and heat capacity (cp_k^o), with two polynomials for two temperature ranges.

$$cp_k^0 \sum_{m=1}^{M} a_{mk} T_k^{(m-1)} \tag{3.7}$$

$$H_k^0 \int_0^{T_k} cp_k^0 dT + H_k^0(0) \tag{3.8}$$

$$S_k^0 \int_{298}^{T_k} \frac{cp_k^0}{T} dT + S_k^0(0) \tag{3.9}$$

where M is the total number of coefficients in the polynomial

Thermodynamics database is also used to declare the elemental composition and the state of the species. Additionally, if required specific heat at constant volume (cv_k^o), internal energy (U_k^o), Gibbs free energy G_k^o and Helmholtz free energy A_k^o is calculated from defined values of S_k^o, H_k^o, cp_k^o. The mixture–averaged molar thermodynamic properties ($\overline{cp}$, $\overline{H}$, $\overline{S}$, etc.) are also calculated from single species thermodynamic properties.

The equilibrium rate constant is calculated from thermodynamic properties assuming ideal gas behavior as follows;

$$K_{ci} = K_{pi} \left(\frac{P_{atm}}{RT}\right)^{\sum_{k=1}^{K} \nu_{ki}} \tag{3.10}$$

$$K_{pi} = e^{\left(\frac{\Delta S_i^0}{R} - \frac{\Delta H_i^0}{RT}\right)} \tag{3.11}$$

where K_{ci} and K_{cpi} are concentration and pressure unit equilibrium rate constants, respectively.

An example of input data format used in CHEMKIN is shown in Figure 3.2. The input file in Figure 3.2 consists of species code, reference, atomic composition, phase,

temperature limits for NASA polynomials, and two seven coefficient NASA polynomial coefficients, (first for higher temperature ranges second for lower temperature ranges).

```
OH                RUS 78O   1H   1          G   200.000  3500.000  1000.000    1
 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11 1.17412376E-14    2
 3.85865700E+03 4.47669610E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06    3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01                   4
H2O               L 8/89H   2O   1          G   200.000  3500.000  1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14    2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01                   4
HO2               L 5/89H   1O   2          G   200.000  3500.000  1000.000    1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14    2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00                   4
```

Figure 3.2. Input data format for Thermodynamic properties

3.4. Transport Properties

Transport properties are also taking a significant role on most of the reacting flow models that are not kinetically limited. It is possible to neglect the transport properties in some cases such as perfectly stirred reactors and closed homogenous reactors, however especially in premixed laminar flames and diffusional flames transport properties may become rate limiting and need to be added. In this study transport properties were also considered in mixture average approach.

Both the mixture-averaged approach (Kee, Warnatz, and Miller 1983) and the full multicomponent approach (Dixon-Lewis 1968) can be used to calculate transport properties. The transport properties database makes the calculations of pure species viscosity, binary diffusion coefficients, pure species thermal conductivities, mass, momentum and energy fluxes, thermal diffusion, and multicomponent or mixture averaged variants of these parameters by using kinetic theory of gases (Hirschfelder, Curtiss, and Bird 1954). For mixtures, mixture-averaged properties or multicomponent properties can be used depending on computational effort.

The equations for the calculation of transport properties are listed below.

Pure species viscosity (η_k);

$$\eta_k = \frac{5}{16}\frac{\sqrt{\pi m_k k_B T}}{\pi \sigma_k^2 \Omega^{(2,2)*}} \tag{3.12}$$

where σ_k Lennard-Jones collision diameter, m_k molecular mass, k_B Boltzmann constant and $\Omega^{(2,2)*}$ collision integral which depends on reduced temperature

$$T_k^* = \frac{k_B T}{\varepsilon_k} \tag{3.13}$$

$$\delta_k^* = \frac{1}{2}\frac{\mu_k^2}{\varepsilon_k \sigma_k^3} \tag{3.14}$$

$$D_{kj} = \frac{3}{16}\frac{\sqrt{2\pi m_k k_B{}^3 T^3 / m_{jk}}}{P\pi\sigma_{jk}^2 \Omega^{(1,1)*}} \tag{3.15}$$

$$m_{jk} = \frac{m_j + m_k}{m_j + m_k} \tag{3.16}$$

The collision integral $\Omega^{(1,1)*}$ depends on reduced temperature (T_k^*), species dipole moments (μ_k) and polarities (α_k)

If both species (k, j) in a binary system are polar or nonpolar;

$$\frac{\varepsilon_{jk}}{k_B} = \sqrt{\left(\frac{\varepsilon_j}{k_B}\right)\left(\frac{\varepsilon_k}{k_B}\right)} \tag{3.17}$$

$$\sigma_{jk}^2 = \frac{1}{2}\left(\sigma_k + \sigma_j\right) \tag{3.18}$$

$$\mu_{jk}^2 = \mu_k \mu_j \tag{3.19}$$

If a polar molecule interacts with a nonpolar molecule;

$$\frac{\varepsilon_{np}}{k_B} = \xi^2 \sqrt{\left(\frac{\varepsilon_n}{k_B}\right)\left(\frac{\varepsilon_p}{k_B}\right)} \tag{3.20}$$

$$\sigma_{np} = \frac{1}{2}\left(\sigma_n + \sigma_p\right)\xi^{-1/6} \tag{3.21}$$

$$\mu_{np}^2 = 0 \tag{3.22}$$

$$\xi = 1 + \frac{1}{4}\alpha_n^* \mu_p^* \sqrt{\frac{\varepsilon_n}{\varepsilon_n}} \tag{3.23}$$

for nonpolar molecule, α_n^* is the reduced polarizability, for polar molecule, μ_p^* is the reduced dipole moment.

$$\alpha_n^* = \frac{\alpha_n}{\sigma_n^3} \tag{3.24}$$

$$\mu_p^* = \frac{\mu_p}{\sqrt{\sigma_n^3 \varepsilon_p}} \tag{3.25}$$

The reduced temperature;

$$T_{jk}^* = \frac{k_B T}{\varepsilon_{jk}} \tag{3.26}$$

Reduced dipole moment;

$$\delta_k^* = \frac{1}{2} \mu_{jk}^{*\,2} \tag{3.27}$$

Species thermal conductivities were assumed as composing of translational, vibrational and rotational contributions (Kee et al. 1986).

$$\lambda_k = \frac{\eta_k}{W_k} (f_{trans} C_{v,trans} + f_{rot} C_{v,rot} + f_{vib} C_{v,vib}) \tag{3.28}$$

$$f_{trans} = \frac{5}{2} \left(1 - \frac{2}{\pi} \frac{C_{v,rot}}{C_{v,trans}} \frac{A}{B} \right) \tag{3.29}$$

$$f_{rot} = \frac{\rho D_{kk}}{\eta_k} \left(1 + \frac{2}{\pi} \frac{A}{B} \right) \tag{3.30}$$

$$f_{rot} = \frac{\rho D_{kk}}{\eta_k} \tag{3.31}$$

$$A = \frac{5}{2} - \frac{\rho D_{kk}}{\eta_k} \tag{3.32}$$

$$B = Z_{rot.} + \frac{2}{\pi} \left(\frac{5}{3} \frac{C_{v,rot}}{R} + \frac{\rho D_{kk}}{\eta_k} \right) \tag{3.33}$$

C_v is the molar heat capacity and it depends on molecular structure (linear/nonlinear).

For linear molecules

$$\frac{C_{v,trans}}{R} = \frac{3}{2} \tag{3.34}$$

$$\frac{C_{v,rot}}{R} = 1 \tag{3.35}$$

$$C_{v,vib} = C_v - 3R \tag{3.36}$$

Translational term for C_v is as follows;

$$C_{v,trans}=\frac{3}{2}R \tag{3.37}$$

For single atoms such as O atom, internal contributions to $C_v$is zero and self-diffusion calculated from next expression;

$$\lambda_k=\frac{\eta_k}{W_k}\left(f_{trans}\frac{3}{2}R\right) \tag{3.38}$$

$$f_{trans}=\frac{5}{2} \tag{3.39}$$

$$D_{kk}=\frac{3}{8}\sqrt{\frac{\pi k_B{}^3T^3/m_k}{P\pi\sigma_k^2\Omega^{(1.1)^*}}} \tag{3.40}$$

Density calculated from ideal gas equation;

$$\rho=\frac{PW_k}{RT} \tag{3.41}$$

where P is pressure and W_k is the species molecular weight.

The rotational relaxation collision number (Z_{rot}) is available at the transport database for 298 K. The temperature dependence of Z_{rot} calculated by following expressions (Parker 1959, Kee et al. 1986);

$$Z_{rot}(T)=Z_{rot}(298)\frac{F(298)}{F(T)} \tag{3.42}$$

and

$$F(T)=1+\frac{\pi^{3/2}}{2}\left(\frac{\varepsilon/k_B}{T}\right)^{\frac{1}{2}}+\left(\frac{\pi^2}{4}+2\right)\left(\frac{\varepsilon/k_B}{T}\right)+\pi^{3/2}\left(\frac{\varepsilon/k_B}{T}\right)^{\frac{3}{2}} \tag{3.43}$$

An example input data format for transport properties is given in Table 3.1.

Table 3.1. Input data format for transport properties

Species Code	Geometry	ε/k_B	σ	μ	α	$Z_{rot}(298)$
H	0	145.000	2.050	0.000	0.000	0.000
H2	1	38.000	2.920	0.000	0.790	280.000
CH4	2	141.400	3.746	0.000	2.600	13.000
H2O	2	572.400	2.605	1.844	0.000	4.000

The geometry (0 for atomic, 1 for linear and 2 for nonlinear), Leannard-Jones potential well depth $\left(\frac{\varepsilon}{k_B}\right)$ (K), The Lennard-Jones collision diameter (σ) (angstrom), dipole moment (μ) (Debye), Polarizability (α) (cubic angstrom), and the rotational relaxation collision number at 298 K $Z_{rot}(298)$ are the input parameters for transport properties (Table 3.1).

The mixture averaged viscosity (η) is calculated from the following semi empirical formula (Bird, Stewart, and Lightfoot 1960).

$$\eta = \sum_{k=1}^{K} \frac{X_k \eta_k}{\sum_{j=1}^{k} X_j \phi_{kj}} \tag{3.44}$$

where

$$\phi_{kj} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_k}{W_j}\right)^{-\frac{1}{2}} \left(1 + \left(\frac{\eta_k}{\eta_j}\right)^{\frac{1}{2}} \left(\frac{W_j}{W_k}\right)^{\frac{1}{4}}\right)^2 \tag{3.45}$$

Mixture averaged thermal conductivity were calculated from the equation below (Wilke 1950).

$$\lambda = \frac{1}{2}\left(\sum_{k=1}^{K} X_k \lambda_k + \frac{1}{\sum_{k=1}^{K} X_k / \lambda_k}\right) \tag{3.46}$$

3.5. Design Equations for Flame Modeling

The design equations that are used to model the premixed, laminar flame are listed below,

- The mass continuity

$$\dot{M} = \rho u A \tag{3.47}$$

- Conservation of Energy (if required);

$$\dot{M}\frac{dT}{dx} - \frac{1}{cp}\frac{d}{dx}\left(\lambda A \frac{dT}{dx}\right) + \frac{A}{cp}\sum_{k=1}^{K} \rho Y_k V_k cp_k \frac{dT}{dx} + \frac{A}{cp} = \sum_{k=1}^{K} \dot{w}_k h_k W_k + \frac{A}{cp}\dot{Q}_{rad} = 0 \tag{3.48}$$

- Species;

$$\dot{M}\frac{dY_k}{dx}+\frac{d}{dx}(\rho A Y_k V_k)-A\dot{w}_k W_k=0 \qquad (k=1, \ldots, K_g) \tag{3.49}$$

- Equation of State;

$$\rho=\frac{P\bar{W}}{RT} \tag{3.50}$$

where;

x : the spatial coordinate

$\dot{M}$: mass flow rate

T : temperature

Y_k : mass fraction of the kth species

$\bar{W}$: mean molecular weight of the mixture

R : universal gas constant

λ : thermal conductivity of the mixture

cp : constant pressure heat capacity of the mixture

cp_k : constant pressure heat capacity of the kth species

$\dot{w}_k$: molar rate of production by chemical reaction of the kth species per unit volume

h_k : specific enthalpy of kth species

V_k : diffusion velocity of kth species

$\dot{Q}_{rad}$: heat loss due to gas and particle radiation

Boundary Conditions;

In the case of burner-stabilized flames $\dot{M}$ is constant. For cold boundary ($x\rightarrow -\infty$) the mass fractions and temperatures are specified as follows;

$$\varepsilon_{k,1}-Y_{k,1}-\left(\frac{\rho A Y_k V_k}{\dot{M}}\right)_{j=1\frac{1}{2}}=0 \tag{3.51}$$

$$T_1-T_b=0 \tag{3.52}$$

$\varepsilon_{k,1}$ is the inlet reactant fractions of the kth species, and T_b is the burner temperature.

At hot boundary ($x\rightarrow \infty$) all the gradients are assumed to be zero.

$$\frac{Y_{k,j}-T_{j-1}}{x_j-x_{j-1}}=0 \tag{3.53}$$

$$\frac{T_j-T_{j-1}}{x_j-x_{j-1}}=0 \tag{3.54}$$

Fixed temperature solution method was used to model the premixed laminar n-heptane flame. Temperature profile was used as an input so that energy equation did not solved for species concentration predictions.

3.6. Theory of Rate of Production and Sensitivity Analysis

Rate of production (ROP) analysis helps us to understand reacting flows by showing net production or consumption contributions of each reaction. The significant reaction pathways can also be seen by doing ROP analysis.

Production of species per unit volume (P_k) is calculated from the equation below (Kee et al. 2006),

$$P_k=\dot{\omega}_k+\sum_{m=1}^{M}\frac{A_m}{V}\dot{S}_{k,m}=\sum_{i=1}^{I}\nu_{ki}q_i \tag{3.55}$$

where ν_{ki} is stoichiometric coefficients for gas phase reactions q_i is rate of progress of gas phase (I) reactions.

The contribution of gas phase reactions on the production of species k is as follows.

$$c_{ki}=\nu_{ki}q_i \tag{3.56}$$

Then the normalized production and destruction of a species can be calculated for each reaction.

Sensitivity analysis is a numerical method to understand effective reactions for several phenomena such as heat release and ignition delay time and species formation. Basically, pre-exponent (A) factors of the reactions multiplied by two then the effect pre-exponent factors are calculated by comparing the solutions. Two solutions are compared to each other, one with original pre-exponent factor and second with changed pre-exponent factor and saved to a solution matrix. Then the normalized sensitivities for each reaction are calculated from the previously saved solution matrixes. This procedure is time consuming especially for the mechanisms that have high amounts of reactions, however it gives excellent information for effective reactions such as rate limiting steps for species formation.

3.7. Target Flame for Modeling

One dimensional, burner stabilized, premixed flames are usually used to develop detailed chemical kinetic mechanisms since the species concentration profiles and temperature depend on just one direction. Systems with one-dimensional dependence are easier to model which result in more precise detailed chemical kinetic model generation. Both consumption pathways for fuels and formation pathways for various species are seen in such flames. At lower distances above the burner, it is possible to see fuel decomposition pathways. At higher distances above the burner, formation pathways of various intermediates and stable species can be investigated. In this work, experimental study of Inal and Senkan, (2002) will be modeled by detailed chemical kinetic modeling technique.

Basically, burner stabilized premixed laminar flat flames can be divided into three zones, pre-flame zone, reaction zone and post flame zone (Figure 3.3). In pre-flame zone, the reactant gas mixture is warmed up from high-temperature downstream gases. The temperature in this zone is lower than upper zones so the reaction rates are slower. At higher regions around the flame (reaction zone), temperature and radical amount are increased so that reactions rates are faster.

When the heat release from reactions are greater than the heat loss from the system, ignition point can be achieved. At the ignition point, chain branching reactions become dominant. Most of the heat release and fuel decomposition occur in this zone. In reaction zone, high temperature and concentration gradients from lower zones provide the self-sustainability of the flame by increasing diffusional heat transfer. In post flame zone, the temperature reaches the maximum and become constant afterward. For fuel-rich flames, the temperature in post flame zone can be lower than the maximum temperature.

The experimental results of Inal and Senkan (2002) (Figure 3.4.) were used to develop a detailed chemical kinetic mechanism for n- heptane oxidation. In that study, the major, minor and trace species had been sampled from height above the burner surface (HAB) by quartz microprobe.

The characterization of the species concentration profiles was done with the help of online sampling line connected to GC/TCD for major gases and GC/MS for minor and trace species.

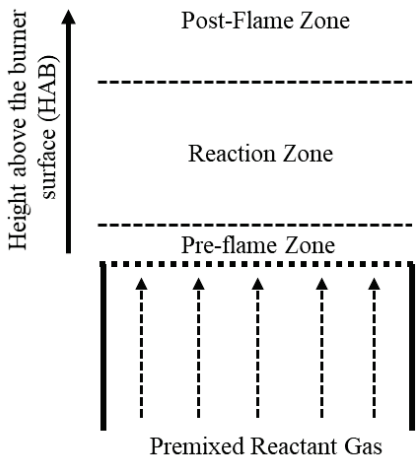

Figure 3.3. Schematic representation for premixed burner stabilized flat flame

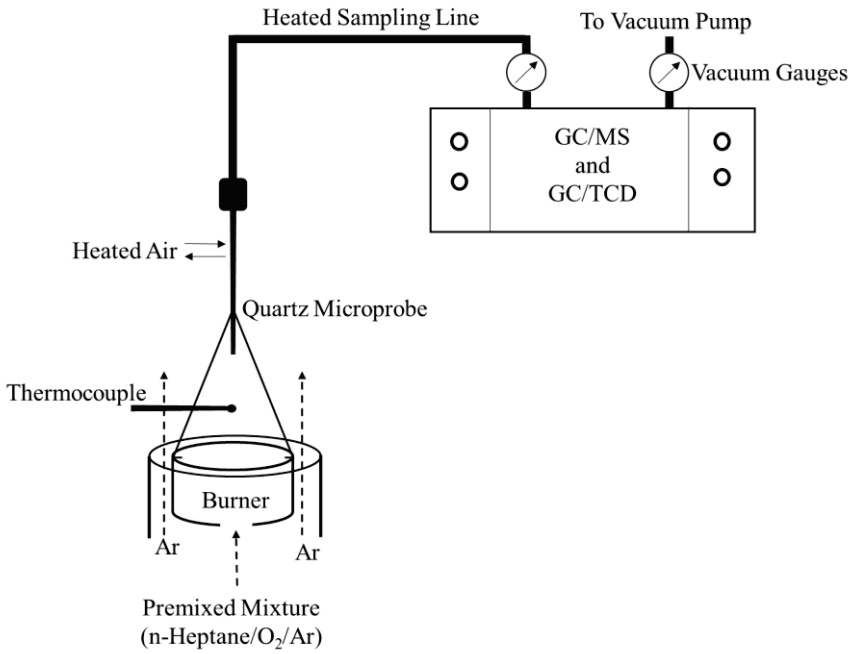

Figure 3.4. Experimental set-up of premixed n-heptane flame (Inal and Senkan 2002)

The study consists of two n-heptane flames with equivalence ratios of 1.97 and 2.10. Argon gas was used to dilute the n-heptane-oxygen mixture in both flames. Additionally, Argon was also used as shield gas to reduce effects of surroundings on the flames. Inlet stream properties for the flame with equivalence ratio of 2.10 are given in Table 3.2. This atmospheric-pressure flame will be the target flame for modeling. Temperature measurements of the flame were done with a silicon oxide-coated Pt-13% Rh/Pt, thermocouple. Rapid injection technique was used for more precise temperature

measurements. However, despite using rapid insertion technique radiation losses from thermocouple junction, especially for soot rich region, require corrections. The temperature measurement corrections will be discussed in the next section.

Table 3.2. Inlet streams properties for Target Flame

Properties	
Initial Velocity (cm/s)	5.17
Equivalence Ratio (ϕ)	2.10
n-Heptane (Mole %)	5.50
O_2 (Mole %)	28.79
Ar (Mole %)	65.71

3.8. Radiation Correction for Flame Temperature Measurement

The high emissivity values for bulk carbon ($\varepsilon \sim 0.95$) results in high temperature loss from an object by radiation since the object act as black body. At fuel-rich flames that phenomena resulted in deviations for temperature measurements when using a thermocouple. The measured temperature from the thermocouple can be different from actual value because soot particles cover the thermocouple junction. Heat loss from thermocouple junction can result in lower temperature measurements than actual flame temperature, especially for soot rich regions. The radiation loss from thermocouple junction can cause up to ~250 K difference between measured temperature and actual temperature if the thermocouple is covered by soot (Boedeker and Dobbs 1988, Chan 2011).

Since the temperature profile of the flame is used as an input for kinetic modeling, it is required to use actual temperatures of gas to achieve more accurate results. The target experimental study reported the measured temperature profiles (Inal and Senkan 2002). It is reported that covered soot particles were cleaned from thermocouple between temperature measurements (Inal 1999). Input temperature profile is highly effective on species concentration (especially for PAHs) predictions of DCKM. Since that, in this section radiation loss corrections for thermocouple measurements will be carried out.

By performing energy balance around a thermocouple junction with an assumption of quasi steady equilibrium resulted in following equation (McEnally et al. 1997).

$$\dot{q}_{convection} = \dot{q}_{radiation} + \dot{q}_{conduction} \tag{3.57}$$

The conduction term can be neglected for thin and long wires ($L_{wire} >> d_{wire}$) (Collis and Williams 1959). Then the equation becomes;

$$\dot{q}_{convection} = \dot{q}_{radiation} \tag{3.58}$$

$$q''_{convection} = \bar{h}(T_{gas} - T_{tj}) \tag{3.59}$$

where, $\bar{h} = \frac{\overline{Nu}_j \times k_{gas}}{d_{tc}}$ and $\overline{Nu}_j = f(Re_d, Pr)$

$$q''_{radiation} = \varepsilon\sigma\left(T_{tj}^4 - T_{surr}^4\right) \tag{3.60}$$

Since $T_{tj} \gg T_{surr}$ the T_{surr} term can be neglected, the final form of energy balance is, (McEnally et al. 1997);

$$\varepsilon_j \sigma T_{tc,j}^4 = \frac{k_{g0} \times Nu_j}{2d_{tc}} \times \left(T_{gas}^2 - T_{tj}^2\right) \tag{3.61}$$

where;

k_{gas}= thermal conductivity of gas (W/mK)

d_{tc}= thermocouple junction diameter

$k_{g0} = \frac{k_g}{T_{gas}}$ = constant; 6.54 x 10^{-5} (W/mK^2)

Nu_j= Nusselt number of thermocouple junction

T_{gas}= gas temperature (K)

T_{tj}= thermocouple junction temperature (K)

σ = Stefan-Boltzmann constant; 5.67x10^{-8} (W/m^2K^4)

ε_j= thermocouple junction emissivity

T_{surr}= surrounding temperature (ambient temperature) (K)

The Nusselt number calculations depend on junction geometry whether it is cylindrical or spherical. The classification of the thermocouple junction is required to be

done by visual characteristics. If the thermocouple junction diameter is distinctly greater than wire diameter the type of the junction is spherical. In this work the type of thermocouple junction is assumed to have spherical geometry ($d_j >> d_{wire}$) as shown in Figure 3.5.

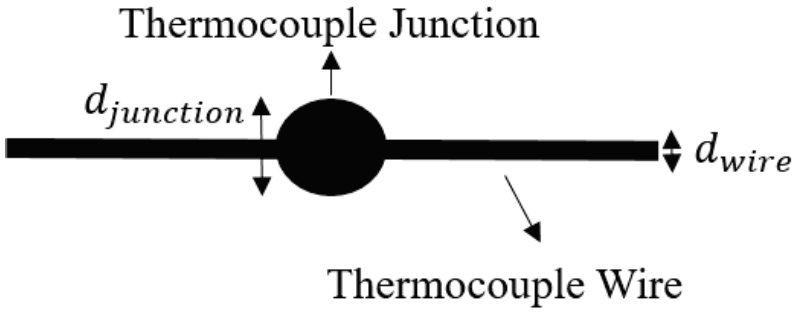

Figure 3.5. Thermocouple junction with spherical geometry

The Nusselt number is calculated from an empirical formula (Acrivos and Taylor 1962) for a single sphere in stokes flow.

$$Nu=2+\frac{1}{2}Pe+\frac{1}{4}Pe^2 lnPe+0.03404Pe^2+\frac{1}{16}Pe^3 lnPe \quad (3.62)$$

$$Pe=Re\times Pr \quad (3.63)$$

The required physical, thermodynamic and transport properties such as gas mixture viscosity, gas mixture thermal conductivity, axial velocity, specific heat and density were obtained from CHEMKIN simulations by using measured temperature profiles with mixture averaged transport properties. DCKM predicts the concentration profiles of major and minor profiles with low error compared to experimental results, so that mixture averaged transport properties were used in Nusselt number calculations are highly accurate.

Predicting the junction emissivity values for sooty flames is major problem for radiation loss corrections on temperature profiles. To predict junction emissivity value, a correlation that assumes linear dependence with junction emissivity with soot volume fraction were used. Since the soot volume fractions were measured experimentally by using light scattering technique (Inal and Senkan 2002), it is possible to predict thermocouple soot coverage by such method. The linear fits for soot volume fractions are shown in Figure 3.6.

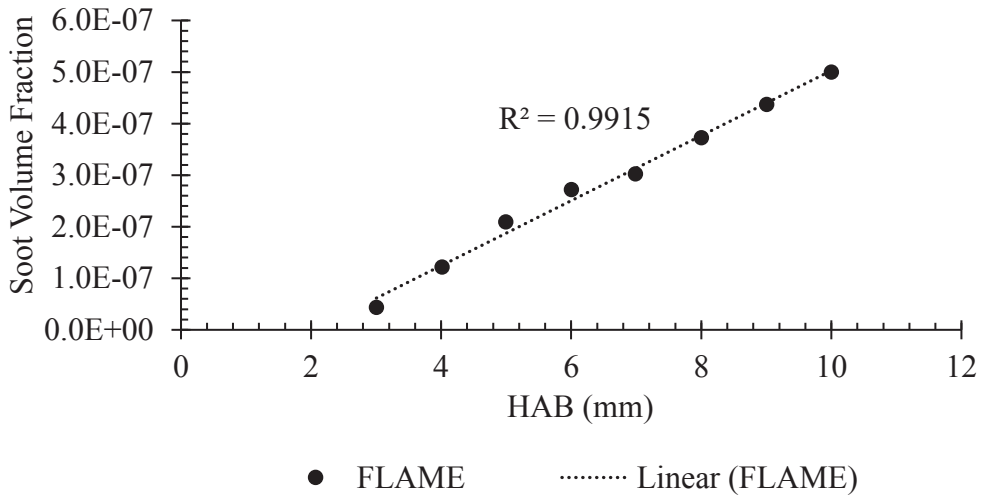

Figure 3.6. Linear fit for soot volume fraction for the flame (Inal and Senkan 2002)

It was reported that thermocouple junction is covered by soot, especially at higher height above the burner (HAB) (Inal and Senkan 2002). It can be assumed that whole thermocouple junction is covered by soot at 10 mm HAB. The maximum emissivity value ($\varepsilon = 0.9$) is achieved at HAB = 10 mm, it is very close to the bulk carbon emissivity. At the burner surface the emissivity value of the thermocouple junction is taken as 0.1 which corresponds to emissivity value of the Pt-13% Rh/Pt, 0.075-mm thermocouple (Omega). Resulting junction emissivity depending on HAB is shown in Figure 3.7.

After solving the energy balance equation given below for gas temperature (T_{gas}) actual temperature for the gas mixture can be achieved. The measured and corrected temperature profiles for the flame are shown in Figure 3.8.

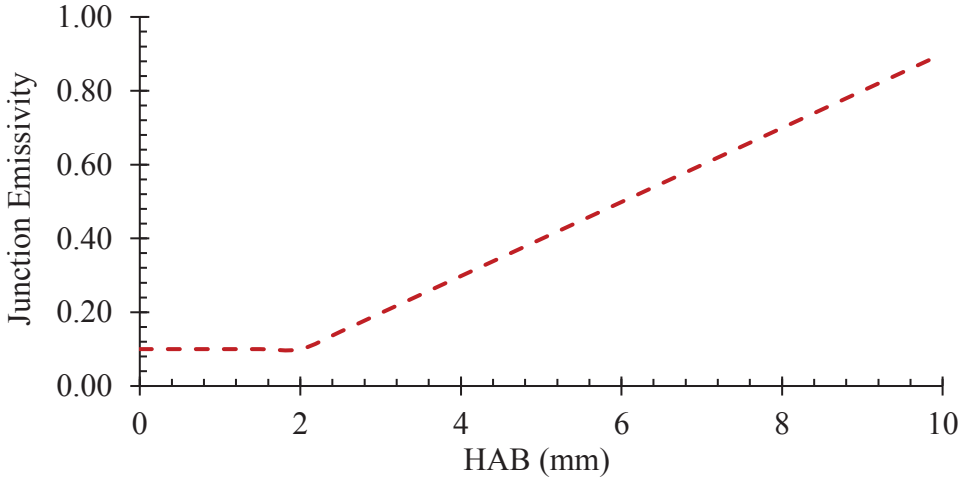

Figure 3.7. Estimated junction emissivity across the flame height

$$\varepsilon_j \sigma T_{tc,j}^4 = \frac{k_{g0} \times Nu_j}{2d_{tc}} \times \left(T_{gas}^2 - T_{tj}^2\right) \quad (3.64)$$

The maximum difference between measured and corrected temperature was 287 K (Figure 3.8). Similar difference between measured and corrected temperatures were observed from different studies in the literature (Boedeker and Dobbs 1988, Chan 2011).

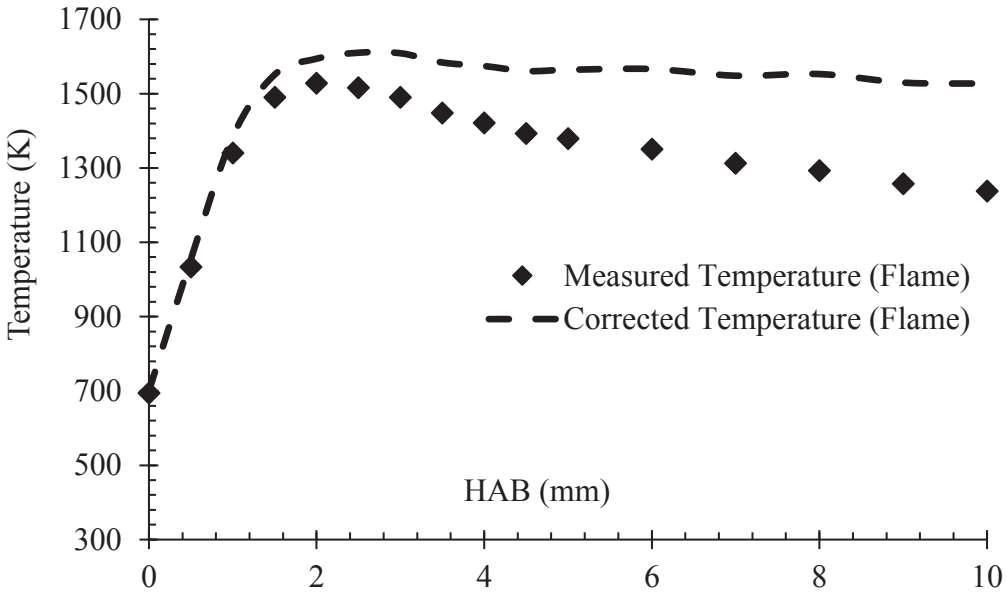

Figure 3.8. Measured and corrected temperature profile for flame

The corrected temperature profile will be used for detailed chemical kinetic modeling. The comparison between some predicted species profiles by using measured and corrected temperature will also be shown in the next chapter.

3.9. Mechanism Generation

At the early stages of mechanism development, available mechanisms in the literature were used to model the flame for the selection of the base mechanism to start mechanism generation. The general characteristics of several n-heptane mechanisms used in mechanism selection are summarized in (Table 3.3). More detailed information was in the literature survey chapter, (i.e. n-heptane oxidation section). The model predictions for species concentration profiles of CH_4, C_2H_2, C_2H_4 and C_3H_6 along with the experimental measurements of Inal and Senkan (2002) were shown in Figure 3.9. – Figure 3.12. respectively.

Table 3.3. General information about n-heptane mechanisms.

Species	Reactions	Information	Reference
218	1223	Mechanism for gasoline surrogate fuels with some PAH formation kinetics	(An et al. 2015)
627	2827	Pure n-heptane mechanism without PAH formation kinetics	(Mehl et al. 2011)
574	3379	High temperature mechanism for gasoline surrogate fuels includes PAH and soot formation kinetics	(Park et al. 2017)
231	1350	Mechanism for Gasoline surrogate fuels with some PAH formation kinetics	(Raj et al. 2012)
> 196	> 6300	Mechanism generated in ethylene flame includes PAH and soot formation kinetics	(Saggese et al. 2015)
1268	5336	Pure n-heptane mechanism without PAH formation kinetics	(Zhang et al. 2016)

Methane mole fraction profile was well-predicted by all mechanisms except Raj et al. (2012) mechanism (Figure 3.9). As seen from Figure 3.10 acetylene experimental profile was underpredicted by all mechanism considered however, mechanism of Mehl et al. (2011) and Saggese et al. (2015) predict the acetylene mole fractions with lower amount of error compared to others.

All mechanisms that are considered predicted the C_2H_4 mole fraction profile for n-heptane flame with low amount of error (Figure 3.11). For C_3H_6 mole fraction predictions mechanisms of Park et al. (2017), Mehl et al. (2011) and Zhang et al. (2016) gave closest results to experimental data (Figure 3.12).

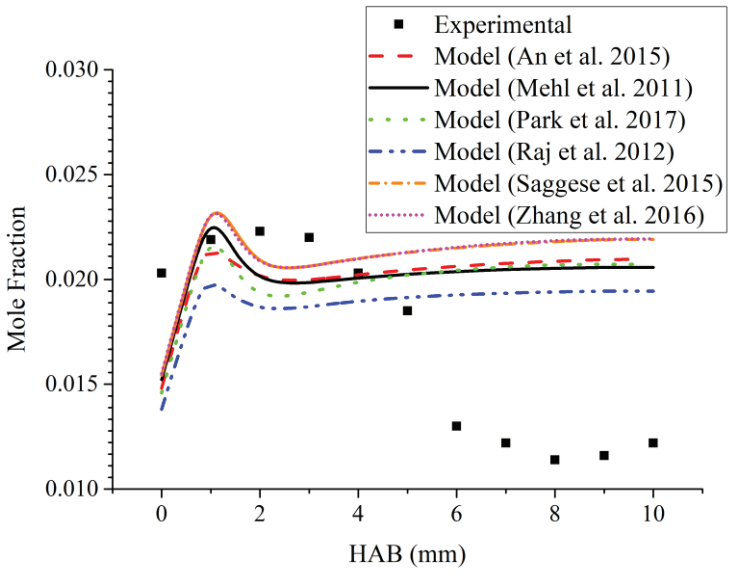

Figure 3.9. Various model predictions for CH_4 profile for flame

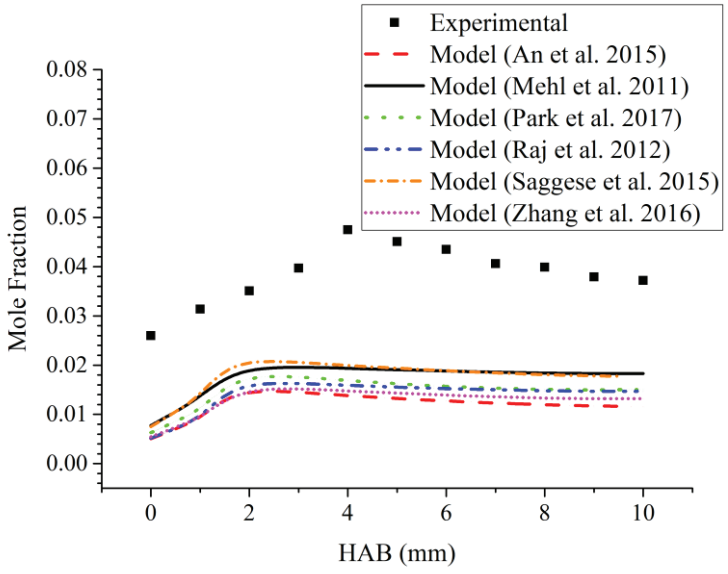

Figure 3.10. Various model predictions for C_2H_2 profile for flame

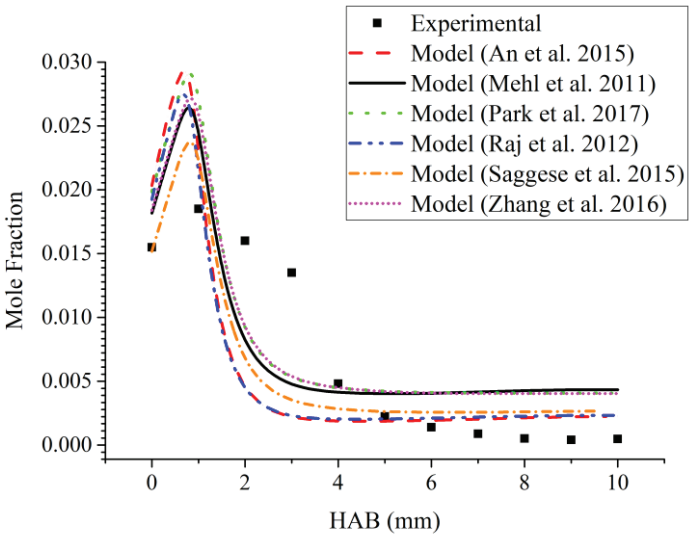

Figure 3.11. Various model predictions for C_2H_4 profile for flame

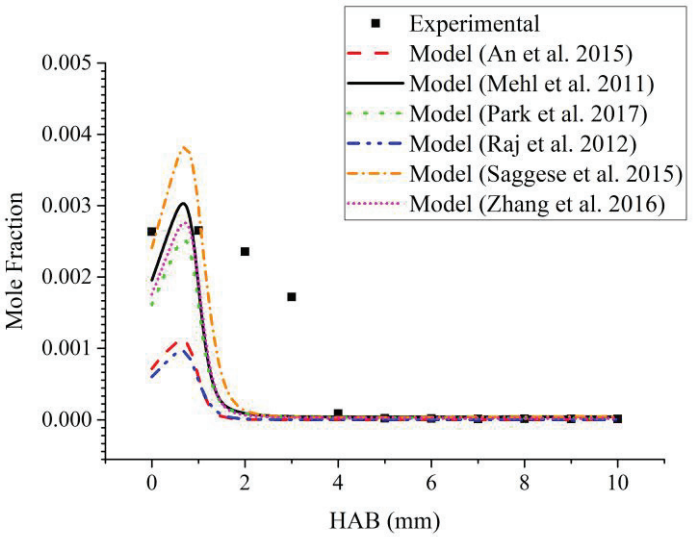

Figure 3.12. Various model predictions for C_3H_6 profile for flame

Those results expressed that Lawrence Livermore National Laboratory (LLNL) n-heptane mechanism (version 3.1) (Mehl et al. 2011) was the most promising mechanism in terms overall precision of the major species. For the generation of the detailed chemical kinetic mechanism for n-heptane flame, base mechanism was chosen as LLNL n-heptane combustion mechanism (version 3.1) (Mehl et al. 2011).

LLNL mechanism was also validated for wide range of conditions in the literature (Hakka et al. 2015, Raj et al. 2012, Park et al. 2017). Moreover, the LLNL n-heptane mechanism was used as the base mechanism on various studies in the literature (Raj et al. 2012, Wang et al. 2015, Park et al. 2017). Additionally, it is a pure n-heptane mechanism

without PAH formation kinetics. So that more arrangements can be done according to target n-heptane flame products and intermediates.

Since the base mechanism did not include either the first aromatic ring and PAH formation, so that donor mechanisms that include PAH formation kinetics were merged with the base mechanism. Mechanisms of Wang and Frenklach (1997), Marinov et al. (1998) and Richter et al. (2000) were the donor mechanisms that were merged with the base mechanism. Since the donor and base mechanisms used different notations to refer species, at the mechanism merging part, the molecular structures of the species were considered. The general information about base and donor mechanisms is given in Table 3.4. As seen from Table 3.4 the total number of reactions and species of base and donor mechanisms are greater than master mechanism. For mutual reactions just one reaction rate parameters were selected from either donor or base mechanism. Detailed information about the master mechanism with all reactions and their rate constant parameters were given in Appendix B as a supplementary material in digital (PDF) format.

Table 3.4. General information about base and donor mechanisms

	# Reactions	# Species	Reference
Base Mechanism	2827	627	(Mehl et al. 2011)
Donor Mechanism 1	553	99	(Wang and Frenklach 1997)
Donor Mechanism 2	672	154	(Marinov et al. 1998)
Donor Mechanism 3	1110	256	(Richter et al. 2000)
Additional Reactions	74	5	(Park et al. 2017)
Master Mechanism	**4185**	**893**	**This study**

Base mechanism involves the consumption pathways of n-heptane excessive amount of alkyl isomers. Decomposition reactions of n-heptane explained by formation of C_1-C_2-C_3-C_4-C_5 and C_6, C_7 alkyls with almost all possible isomers, in the base mechanism.

Aromatic ring and some PAH species formation pathways with HACA growth was involved in the mechanism of Wang and Frenklach (1997) (donor mechanism 1).

Additional linear PAH (anthracene), angular PAH (phenanthrene) formation and branched aromatic (indene, cyclo-penta[cd]pyrene etc.) formation pathways were involved in the mechanism of Marinov et al. (1998), (donor mechanism 2). Detailed formation and oxidation pathways of high molecular weight PAH species (Anthracene, aceanthrylene, cyclopenta[cd]pyrene, chrysene, etc.) were involved in the mechanism of Richter et al. (2000), (donor mechanism 3). Additional PAH and intermediate formation reactions were also added from the recent study of Park et al. (2017).

Additionally, if available, reaction rate parameters of sensitive reactions on the formation of several species were updated. It is possible to have high amount of uncertainty on elementary/nonelementary rate constant measurements/calculations. So that, for the reactions that have high amount of uncertainty on rate parameters, it is hard to decide which rate constant parameters are the best for the system of interest. Sensitivity analysis is one way to find out the reactions that have most effect on the formation of selected species. Sensitivity analysis for acetylene is shown that most sensitive reactions for the formation and decomposition of acetylene are as follows (see Appendix A, Figure A. 1);

$C_2H_2 + O = H + HCCO$ (negative sensitivity)

$C_2H_3 + O_2 = O + CH_2CHO$ (negative sensitivity)

$C_2H_2 + O = CH_2 + CO$ (negative sensitivity)

For the first and third reactions the forward reactions are decomposition pathways for acetylene. The decrease in forward rate constants of $C_2H_2 + O = CH_2 + CO$ and $C_2H_2 + O = H + HCCO$ results in increase for the acetylene mole fractions. As mentioned previously acetylene was underpredicted from the base mechanism so that lower rate constant parameter was required to improve model predictions. Additionally, the forward reaction of $C_2H_3 + O_2 = O + CH_2CHO$ was also required to be decreased to improve acetylene model predictions on the flame since C_2H_3 was the main intermediate that forms acetylene. Various rate constant parameters were published for the reactions that found to be sensitive for acetylene formation. Those reaction rate parameters are listed in Figure 3.13, Figure 3.14 and Figure 3.15.

As seen from Figure 3.13 the modified Arrhenius fit rate constants parameters that proposed from Tsang and Hampson (1986) is the lowest forward rate constant within the

uncertainty range. The rate parameters for $C_2H_2 + O = H + HCCO$ of the base mechanism were changed with Tsang and Hampson (1986).

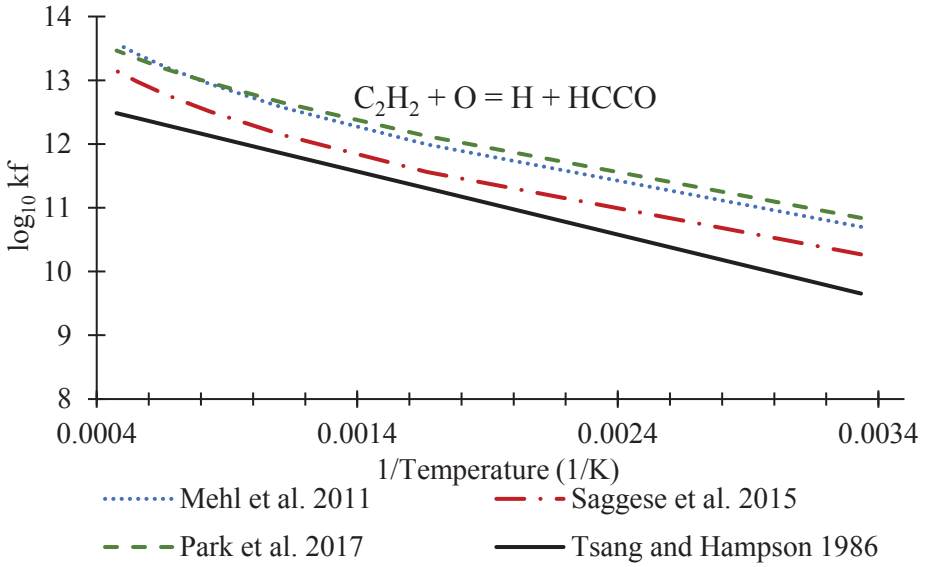

Figure 3.13. Forward logarithmic rate constant versus inverse temperature for C_2H_2+O=HCCO+H reaction from different sources.

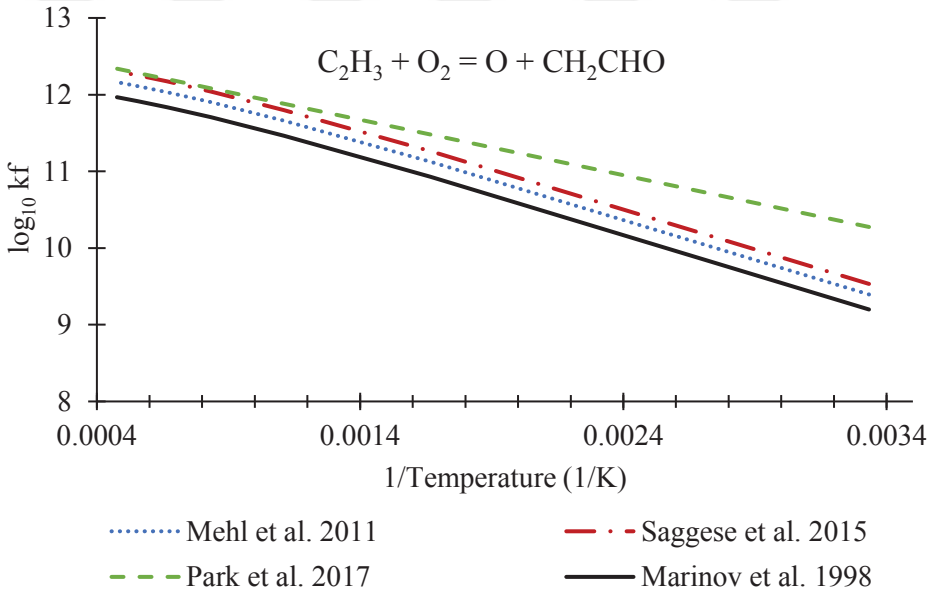

Figure 3.14. Forward logarithmic rate constant versus inverse temperature for C_2H_3+O_2=O+CH_2CHO reaction from different sources.

Available rate parameters for the reaction $C_2H_3 + O_2 = O + CH_2CHO$ is shown in Figure 3.14. The rate parameters proposed from Marinov et al. (1998) were used to improve the model predictions on the flame. The modified Arrhenius plots for C_2H_2+O =

CH_2+CO reaction shows that the rate parameters that suggested by Saggese et al. (2015) are the lowest forward rate constant (Figure 3.15).

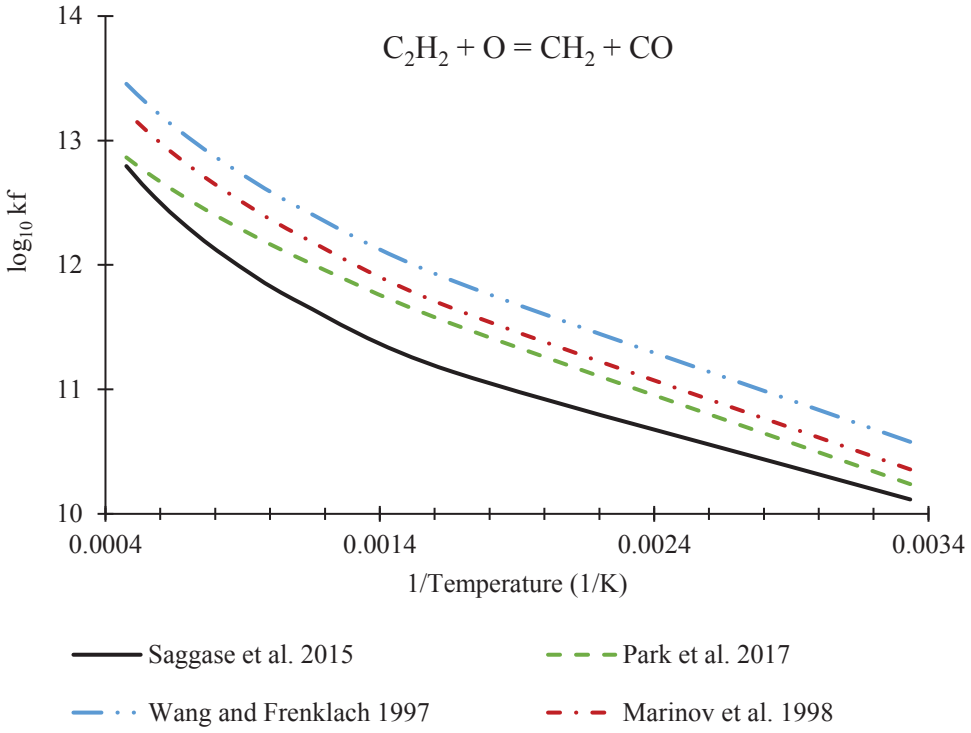

Figure 3.15. Forward logarithmic rate constant versus inverse temperature for C_2H_2+O=CH_2+CO reaction from different sources.

The rate parameters of base mechanism for C_2H_2+O = CH_2+CO reactions were altered with the ones from Saggese et al. (2015) to improve model predictions of C_2H_2 on flames.

Similar methods were used to improve model predictions for the reactions listed in Table 3.5. Depending on the sensitivity analysis alternative rate constants were investigated for those reactions.

Reaction rate parameters suggested from Wang and Frenklach (1997) were used for $C_2H_4 + H = C_2H_3 + H_2$ reaction since it's Arrhenius fit corresponds to higher forward rate constant at high temperatures, (Figure 3.16). Additionally, reaction rate parameters listed in Table 3.5 were changed.

In addition to changes were done to base mechanism some reaction rate parameters in the donor mechanisms were also changed to available up-dated reaction rate parameters from the literature by doing the sensitivity analysis on overestimated/underestimated species mole fractions profiles (see Appendix A).

As seen from Figure 3.17 there is high uncertainty for this reaction since the suggested rate parameters are highly different from each other. The rate constant parameters of Wang et al. (2015) were used.

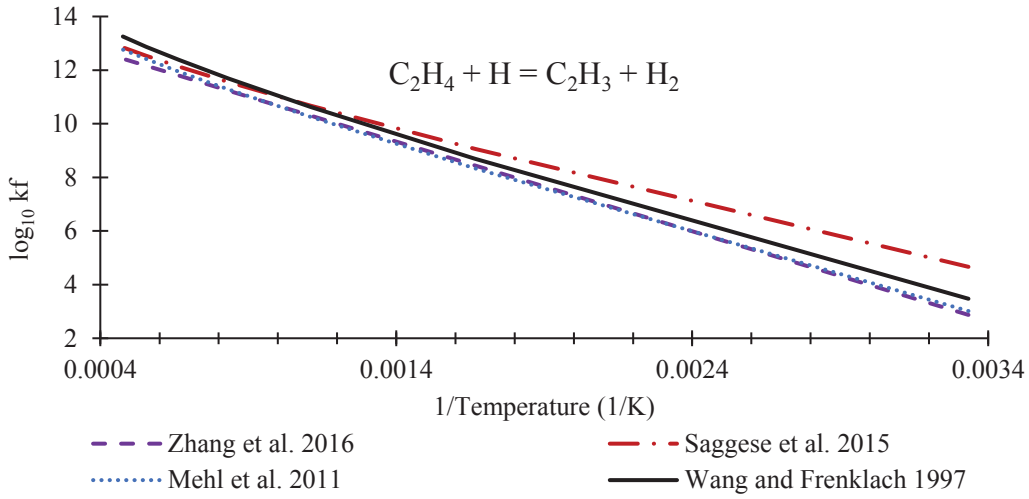

Figure 3.16. Forward logarithmic rate constant versus inverse temperature for $C_2H_4 + H = C_2H_3 + H_2$ reaction from different sources.

Table 3.5. Altered Rate constant parameters from base mechanism

Reactions	A (mol, cm, s units)	ß	Ea (cal/mol)	Reference
H+O2=O+OH	1.04E+14	0	15286	(Zhang et al. 2016)
C3H5-A+H=C3H4-A+H2	5.00E+13	0	0	(Marinov et al. 1998)
C3H5-A+CH3=C3H4-A+CH4	3.02E+12	-0.32	-1.31E+02	(Marinov et al. 1998)
C3H4-A+CH3=C3H3+CH4	1.50E+00	3.5	5.60E+03	(Marinov et al. 1998)
C3H3+H+(M)=C3H4-P(+M)	1.66E+15	-0.37	0	(Marinov et al. 1998)
C2H+CH3=C3H4-P	8.00E+46	-10	4.63E+04	(Richter et al. 2000)
C3H3+O=CH2O+C2H	7.17E+13	0	0.00E+00	(Richter et al. 2000)
C3H3+OH=C3H2+H2O	2.00E+13	0	8.00E+03	(Park et al. 2017)
C3H3+H=C3H2+H2	2.14E+05	2.52	7.45E+03	(Park et al. 2017)
C2H4+H=C2H3+H2	1.33E+06	2.53	1.22E+04	(Wang and Frenklach 1997)
C2H2+O=CH2+CO	3.50E+03	2.8	5.00E+02	(Saggese et al. 2015)
C2H3+O2=O+CH2CHO	3.50E+14	-0.611	5.26E+03	(Marinov et al. 1998)
C2H2+O=H+HCCO	9.03E+12	0	4.53E+03	(Tsang and Hampson 1986)

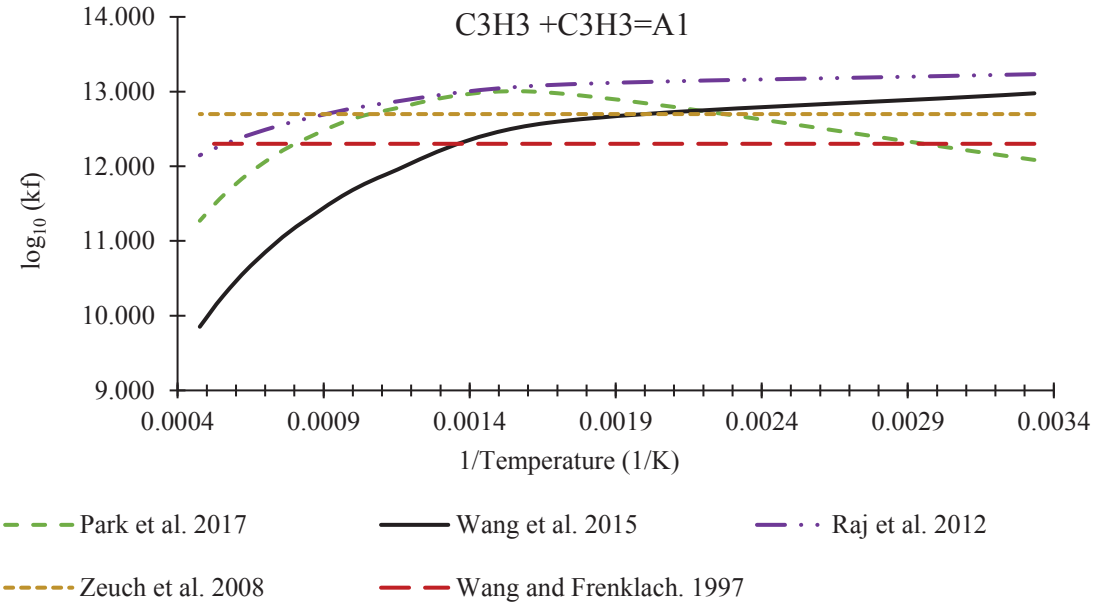

Figure 3.17. Forward logarithmic rate constant versus inverse temperature for $C_3H_3 + C_3H_3$=A1 reaction from different sources.

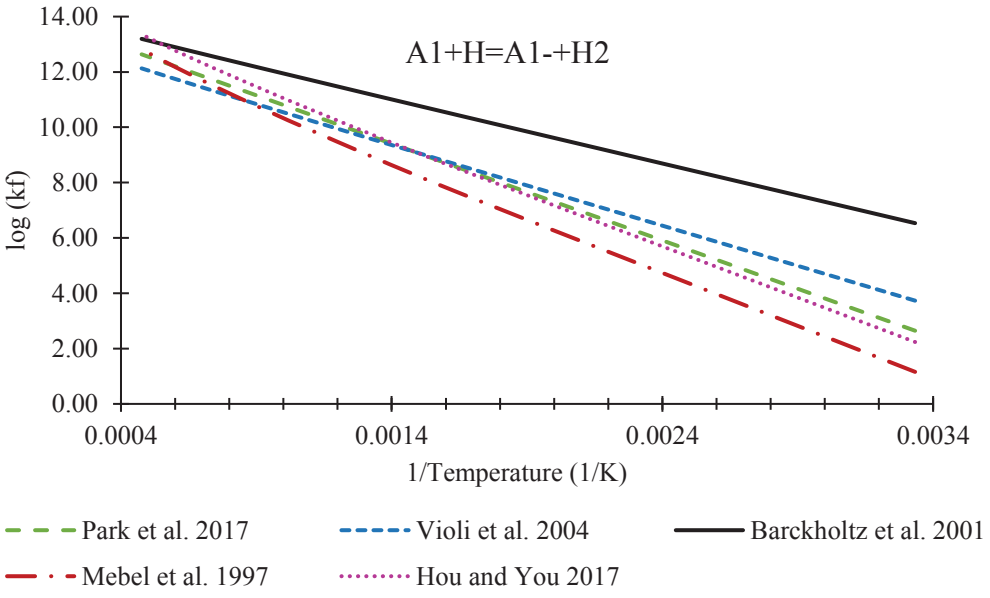

Figure 3.18. Forward logarithmic rate constant vs inverse temperature for A1+H=A1-+H_2 reaction from different sources.

Rate constant parameters of Barckholtz et al. (2001) were used for hydrogen abstraction reaction from benzene (A1+H=A1-+H2). The hydrogen abstraction from the collision with H radical (Figure 3.18) needs to be analogous with reverse hydrogen abstraction reaction with the collision with methyl radical (CH_3) (Figure 3.19). To improve model predictions of benzene depending on sensitivity analysis (see Appendix

A), rate constant parameters of Park et al. (2017) were used for the A1-+CH_4=A1+CH_3 reaction.

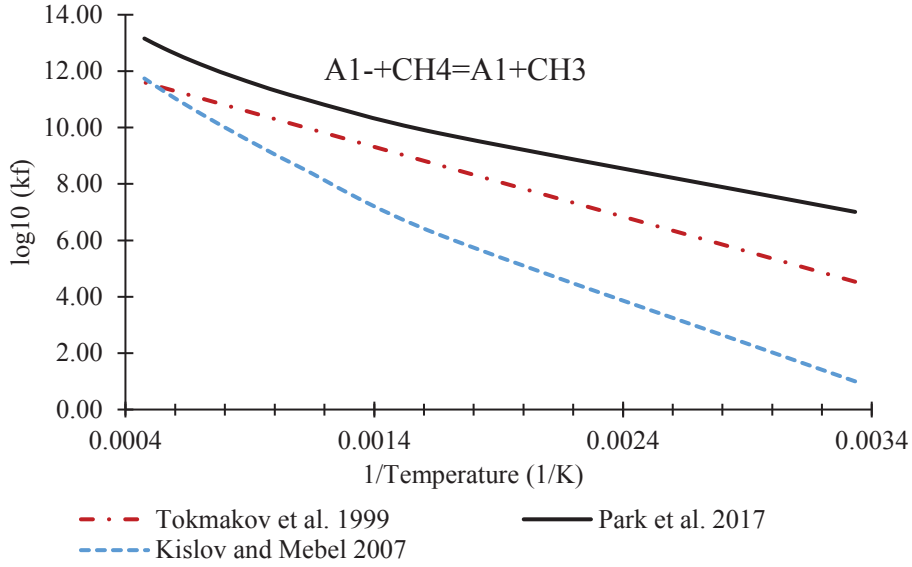

Figure 3.19. Forward logarithmic rate constant vs inverse temperature for A1-+CH4=A1+CH3 reaction from different sources.

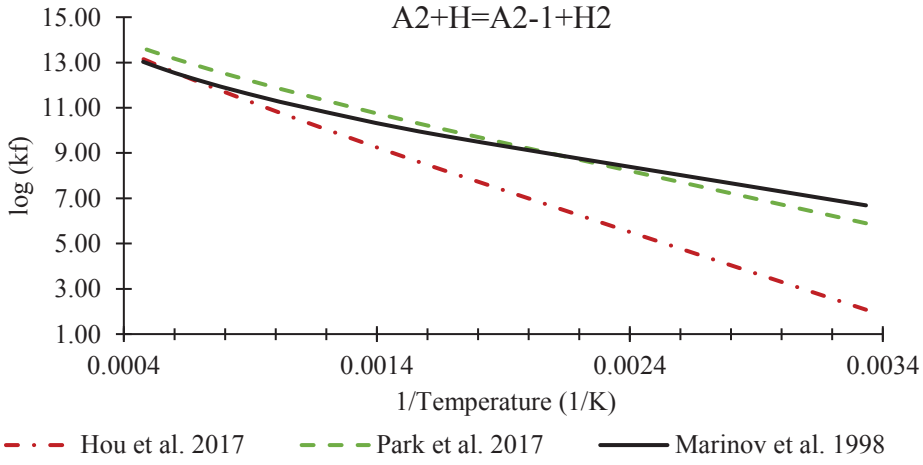

Figure 3.20. Forward logarithmic rate constant vs inverse temperature for A2+H=A2-1+H2 reaction from different sources.

For the H abstraction reaction from naphthalene (A2), A2+H=A2-1+H_2 rate constant parameters from Marinov et al. (1998) were used.

CHAPTER 4

RESULTS AND DISCUSSION

4.1. Validations of the Mechanism

To determine the capabilities of the master mechanism, different sets of experimental data from various studies were modeled. This procedure is called as mechanism validation. Species concentration profiles were validated by experimental data of jet stirrer reactor (JSR) (Hakka et al. 2015, Zhang et al. 2016) and premixed laminar flame (Bakali, Delfau, and Vovelle 1998). Shock-tube experimental data (Zhang et al. 2016) were used to validate the master mechanism in terms of ignition delay time estimations. The experimental conditions of the JSR studies that were used in the mechanism validation part is given in Table 4.1. Helium (He) was the inert gas to keep temperature constant for those experiments.

Table 4.1. Experimental conditions of JSR studies

Conditions	**(Hakka et al. 2015)**	**(Zhang et al. 2016)**
Reactor Volume (cm^3)	86.5	95
Temperature (K)	550 to 1100	500 to 1100
Pressure (torr)	800	800
Residence time (s)	2	2
Equivalence Ratio (Φ)	3	2
Inlet He fraction (mol %)	0.977	0.968
Inlet O_2 fraction (mol %)	0.018	0.027
Inlet n-C_7H_{16} fraction (mol %)	0.005	0.005

Experimental mole fractions of n-heptane, acetylene (C_2H_2), propadiene (C_3H_4) and benzene (C_6H_6) were taken from those two JSR studies (Hakka et al. 2015, Zhang et al. 2016) and they were used for mechanism validation. The spherical JSRs were assumed as perfectly stirred (0-dimensional flow) reactor with fixed temperature. Transient solver with an end time same as the residence time were used to model JSR studies. The inlet stream properties were kept constant except the temperatures for each JSR. For every

temperature new run were made with the change of reactor temperature and inlet stream temperature to draw temperature versus species mole fractions profiles.

The master mechanism slightly underestimated the low temperature (500 K to 700 K) n-heptane mole fractions, for both equivalence ratios. However, for the negative temperature coefficient region (~700 K to ~850 K) and higher temperatures, the difference between the experimental data and model predictions were small (Figure 4.1).

As seen from Figure 4.2 the master mechanism overpredicted acetylene mole fractions with a factor of about 3 for both JSR studies, yet the formation temperature of acetylene was properly estimated (~ 850 K). Low temperature (550 K to 700 K) formation of propadiene which resulted from n-heptane conversion was estimated by the master mechanism (Figure 4.3). However, the experimental measurements did not involve propadiene formation up to ~850 K for both equivalence ratios (i.e. 2 and 3). There were sharp increases for propadiene mole fractions at ~875 K for master mechanism predictions however, peaks were not reported experimentally for both equivalence ratios. For temperatures greater than 900 K the master mechanism predictions were very close to the JSR experimental data especially for equivalence ratio of 2. As seen from Figure 4.4, master mechanism slightly overestimated the formation of propane at temperatures between 800 K to 1100 K.

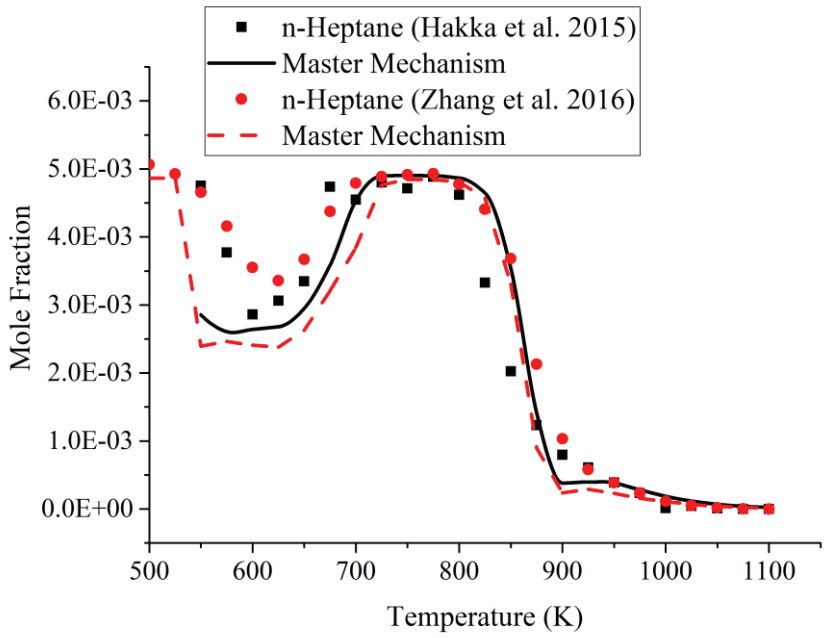

Figure 4.1. Validation of the master mechanism on n-heptane mole fraction with JSR

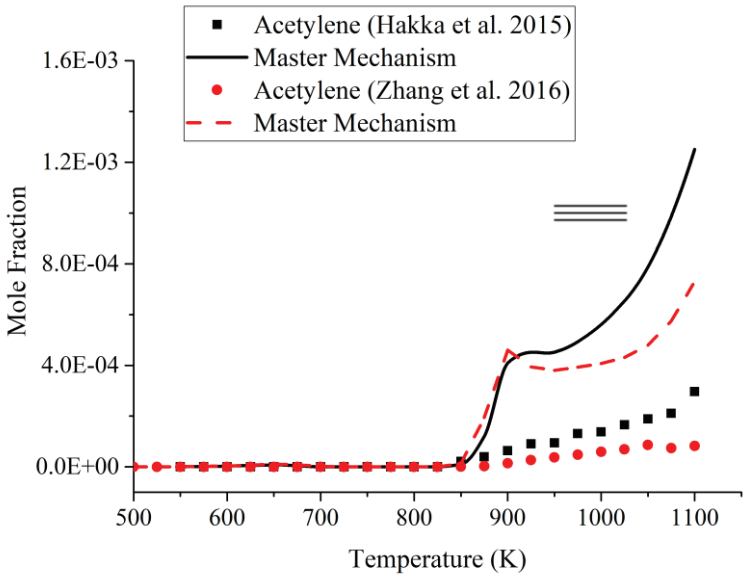

Figure 4.2. Validation of the master mechanism on acetylene mole fraction with JSR

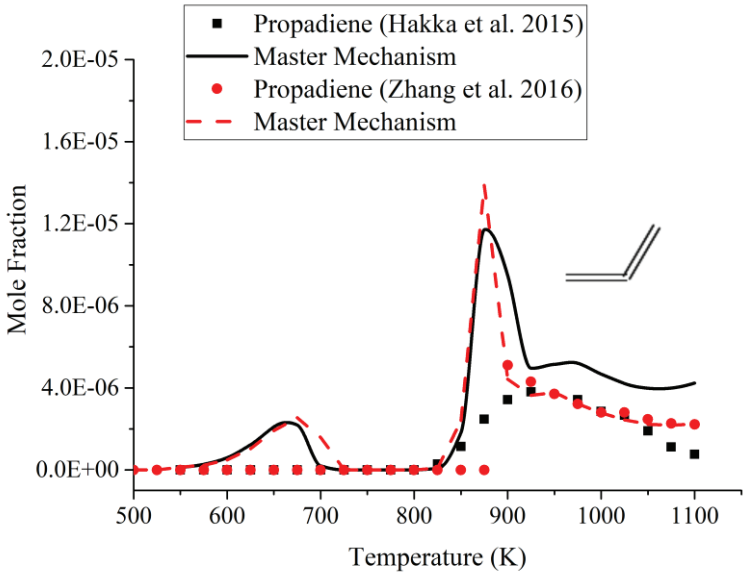

Figure 4.3. Validation of the master mechanism on propadine mole fraction with JSR

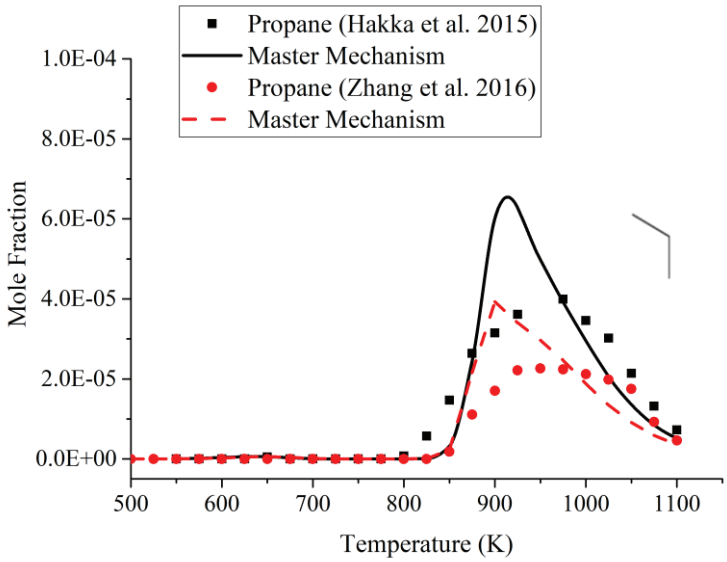

Figure 4.4. Validation of the master mechanism on propane mole fraction with JSR

Model predictions for benzene mole fractions were consistent with the experimental data at equivalence ratio of 2 (Figure 4.5.). For equivalence ratio of 3, the master mechanism could not predict the low temperature (550 K to 850 K) formation of benzene.

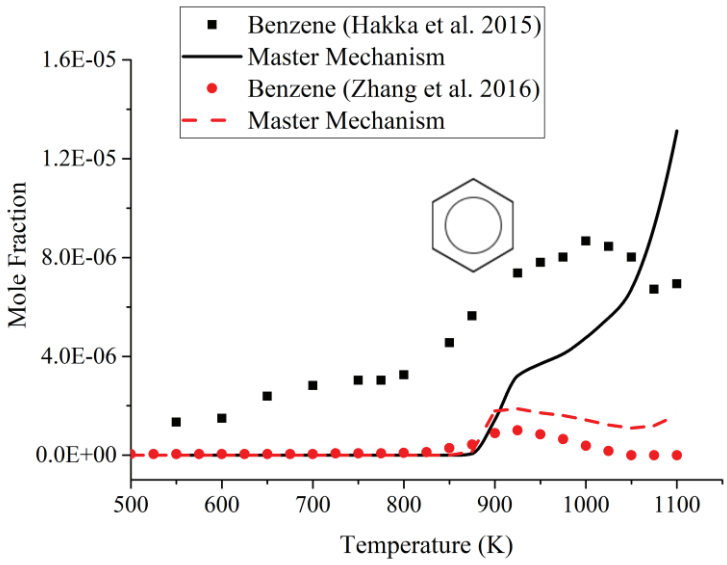

Figure 4.5. Validation of the master mechanism on benzene mole fraction with JSR

From the validations of the master mechanism with jet stirred reactor, it can be said that the master mechanism is more capable of mole fraction predictions at the equivalence of 2. However, the uncertainties of both temperature and mole fraction measurements should also needed to be consider.

Additional model validation was done by one dimensional atmospheric-pressure premixed laminar flame of Bakali et al. (1998). The inlet stream properties of the flame were given in Table 4.2. The flame was modeled with fixed temperature solver based on the measured temperature profile. N_2 was used as carrier gas for n-heptane but the study did not report any NO_x measurements.

Experimental mole fractions of C_2 species (acetylene, ethylene, ethane) with model predictions are given in Figure 4.6. Except for the shift to the burner surface (HAB = 0) of about 1.2 mm, all C_2 species concentrations were predicted with low error. Other modeling studies (Park et al. 2017, An et al. 2015) that modeled the premixed n-heptane flame of Bakali et al. (1998) also reported similar shift as ~1.2 mm on their results. Since all species are shifted together, Figure 4.6, Figure 4.7 and Figure 4.8 were drawn by moving the model results to right side by 1.2mm. Since the estimated profiles were shifted to the right side, there were no solution for HAB less than 1.2mm As seen from Figure 4.6, Figure 4.7 and Figure 4.8.

Acetylene, ethylene and ethane species mole fraction were predicted by master mechanism with very low error comparing with the experimental data. From Figure 4.7, it can be seen that, master mechanism overpredicted the diacetylene mole fraction profile with a factor of about 3. However, the master mechanism gave proper results for the vinylacetylene mole fraction profile.

Benzene mole fraction profile across the flame height can be seen from Figure 4.8. Master mechanism under-estimated the benzene mole fraction with an error less than factor of 2 for most height above the burner surface. The peak corresponding to HAB = 2 mm was predicted by the mechanism, however the measured peak was greater than the estimated one.

Table 4.2. Inlet stream properties for flame

Properties	**(Bakali, Delfau, and Vovelle 1998)**
Initial Velocity (cm/s)	4.98
Equivalence Ratio (ϕ)	1.9
n-Heptane (Mole %)	3.98
O_2 (Mole %)	23.01
N_2 (Mole %)	73.01

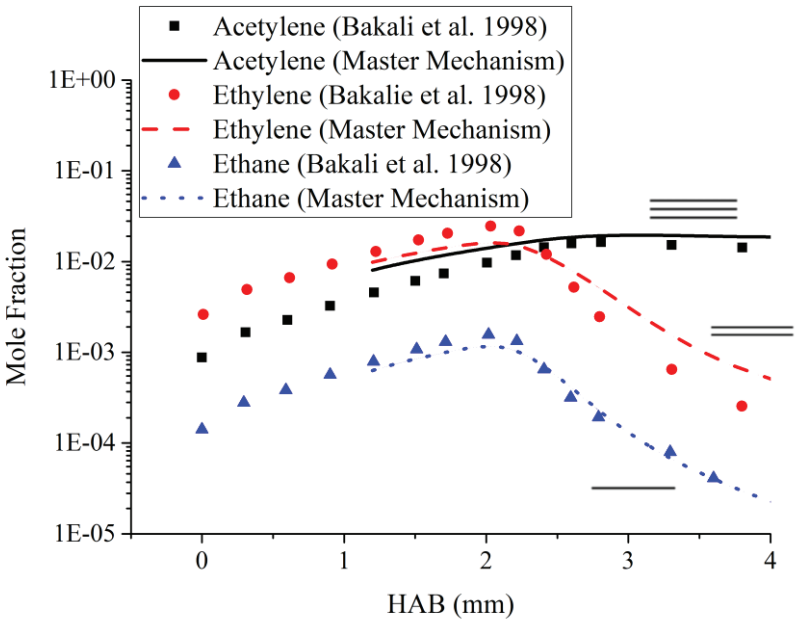

Figure 4.6. Validation of the master mechanism on C_2 species mole fraction profiles of a Flame.

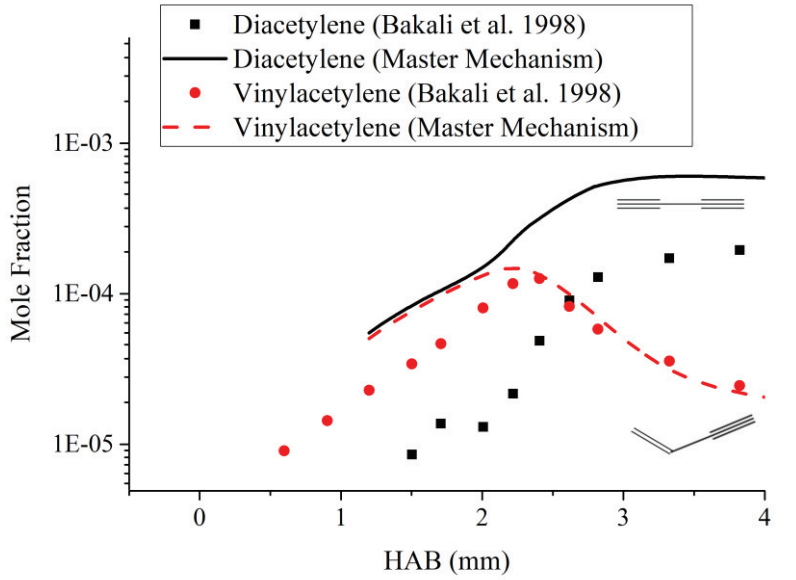

Figure 4.7. Validation of the master mechanism on diacetylene and vinylacetylene mole fraction profiles of a Flame.

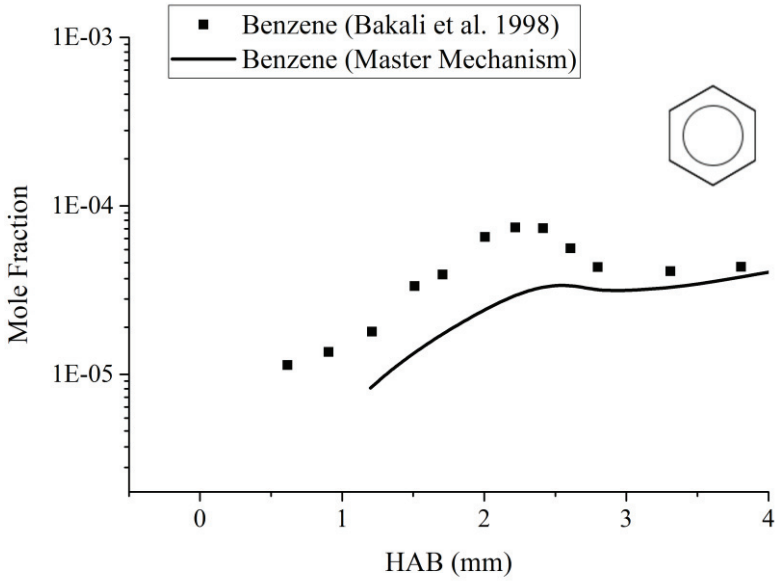

Figure 4.8. Validation of the master mechanism on benzene mole fraction profiles of a Flame

Additional validations were done to understand the capabilities of the master mechanism in terms of ignition delay time. Ignition delay time can be defined as, the time required to see the rapid temperature increase that caused from the ignition for a fuel-oxidizer mixture. Two shock tube studies were used for model validation by ignition delay. The details of the experimental conditions are given in Table 4.3 Constant volume, closed homogenous batch reactor were used in the modeling. Similar with rapid compression machine, isentropic compression and expansion were assumed, and non-reactive pressure time trace were input as effective volume change (Zhang et al. 2016).

Table 4.3. Shock tube experimental data used in mechanism validations in terms of ignition delay time

Conditions	**(Zhang et al. 2016)**	**(Zhang et al. 2016)**
Temperature (K)	726 to 1412	755 to 1150
Pressure (bar)	~20	~38
Equivalence Ratio (Φ)	1	1
Reactant N_2 fraction	0.775	0.775
Reactant O_2 fraction	0.206	0.206
Reactant n-C_7H_{16} fraction	0.019	0.019

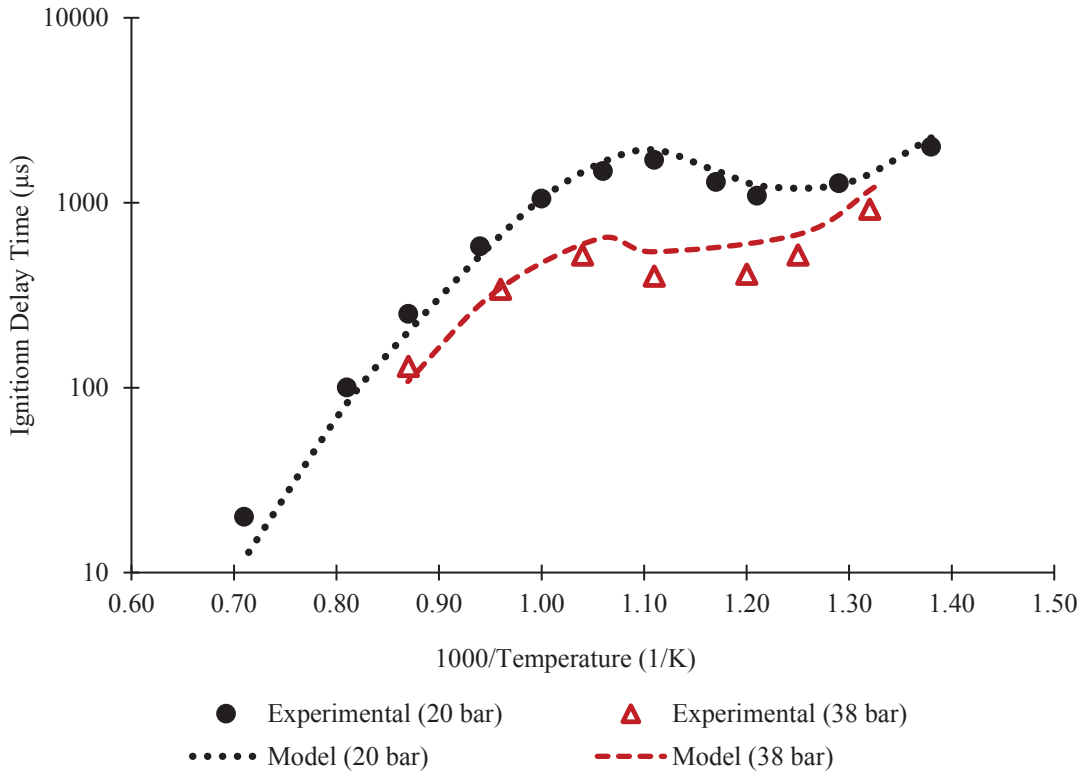

Figure 4.9. Validations of the master mechanism by ignition delay time

As seen from Figure 4.9, for 20 bar pressure, master mechanism predicted the ignition delay times with low error on a wide temperature range (726 K to 1412 K). There was an underestimation around a factor of 1.5 at highest temperature. For 38 bar pressure, master mechanism overestimated the ignition delay time around 40 % more than the experimental values for temperatures from 750 K to 950 K. Validations of the master mechanism with shock tube experimental data were shown that, the master mechanism was able to predict ignition delay times at similar conditions to the gasoline engine operating conditions.

To understand the effect of temperature corrections on the model predictions at the target flame (Inal and Senkan 2002), comparison of some species mole fractions predictions with corrected and measured temperature were carried out.

As seen from Figure 4.10. there was very small difference between n-heptane mole fraction predictions using measured and corrected temperature profile. Temperature corrections were slightly increased hydrogen mole fractions of the model predictions (Figure 4.11), this could be caused from increase in the reaction rates of hydrogen abstraction reactions.

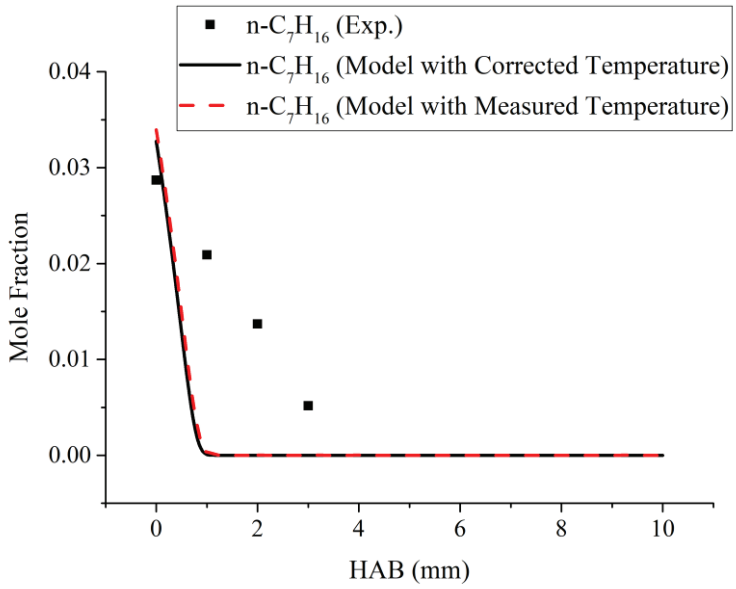

Figure 4.10. Effect of temperature profile to n-heptane mole fraction

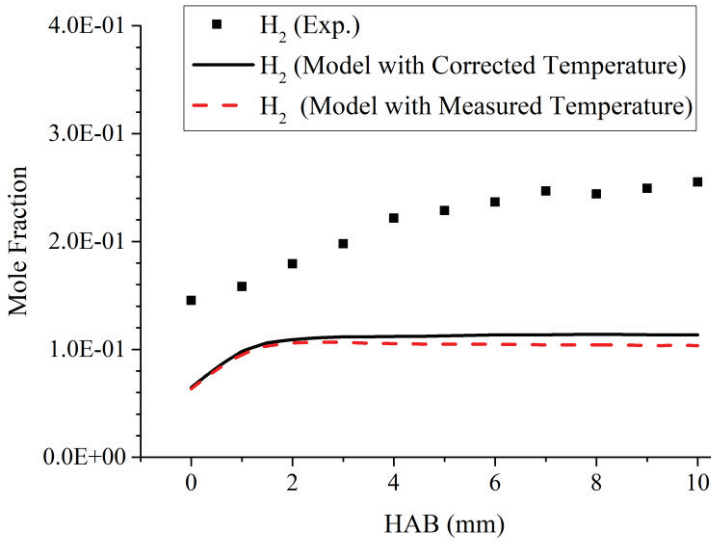

Figure 4.11. Effect of temperature profile hydrogen mole fraction

For methane mole fraction profile, the effect of temperature correction was greater than the previously mentioned species. CH_4 mole fraction predictions were decreased with the use of corrected temperature profile (Figure 4.12). The amount of decrease in the CH_4 mole fraction predictions was greater for higher HAB.

For acetylene (Figure 4.13), benzene (Figure 4.14) and naphthalene (Figure 4.15) the effects of temperature correction on the mole fraction profiles were very low. Acetylene mole fraction predictions were slightly increased when using corrected

temperature profile as seen from Figure 4.13. especially for higher heights above burner surface (HAB > 3 mm).

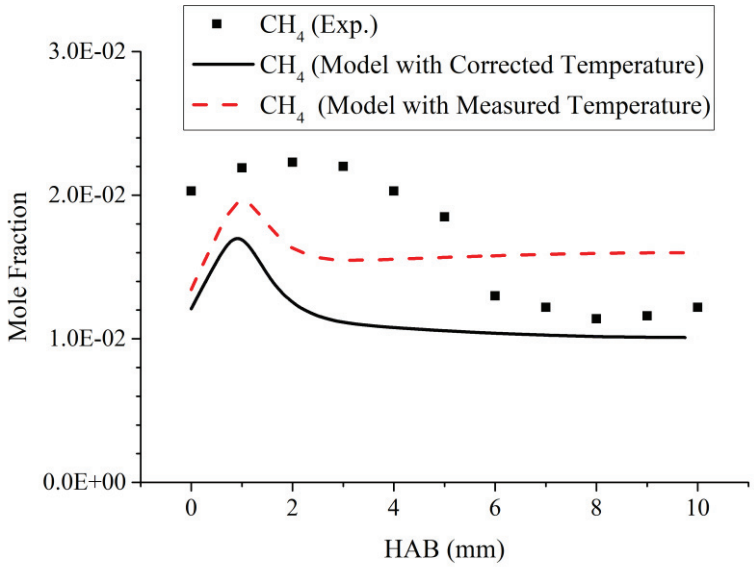

Figure 4.12. Effect of temperature profile to methane mole fraction

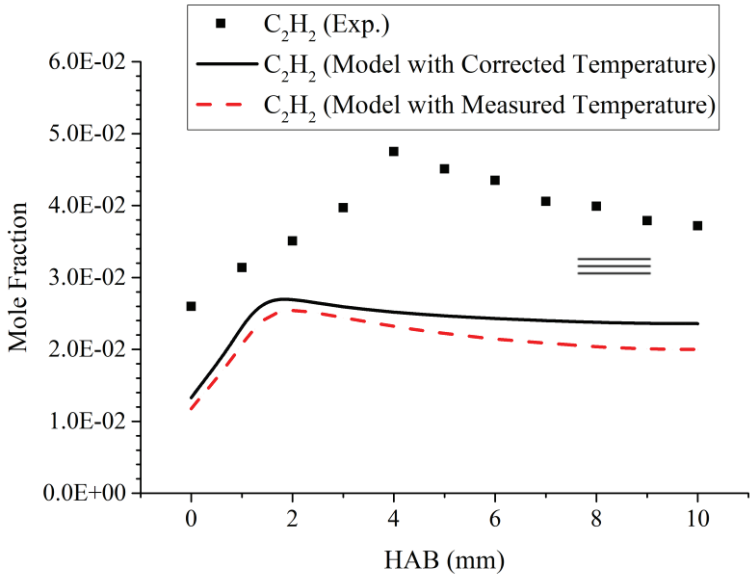

Figure 4.13. Effect of temperature profile to acetylene mole fraction

Using corrected temperature instead of measured temperature profile almost did not affect the benzene mole fraction predictions except for the slight increase at lower heights above the burner surface (HAB < 2 mm) (Figure 4.14). As seen from Figure 4.15. For naphthalene there were slight decreases for 3 mm < HAB < 6 mm with corrected

temperature profile. however, modeling with corrected temperature resulted to higher naphthalene mole fraction for HAB > 7 mm (Figure 4.15).

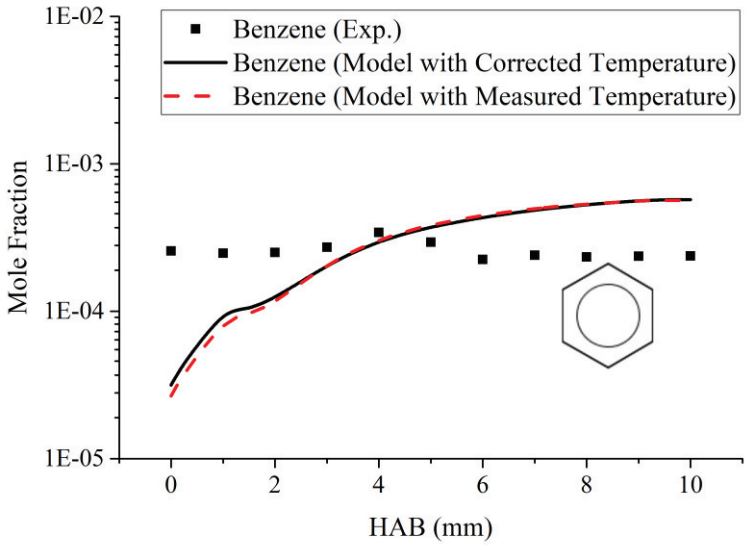

Figure 4.14. Effect of temperature profile to benzene mole fraction

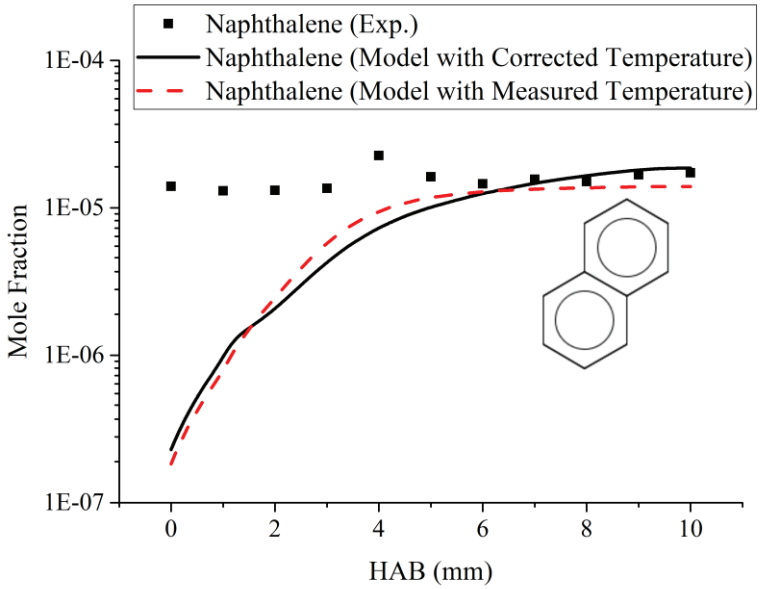

Figure 4.15. Effect of temperature profile to naphthalene mole fraction

As seen from Figure 4.16, input temperature profile had significant effects on the toluene mole fraction predictions. Especially for HAB greater than 2 mm, model predictions were decreased with corrected temperature profile. For HAB greater than 2 mm the temperature difference between measured and corrected temperature profile was

greater as seen from Figure 3.8. It can be said that toluene mole fraction predictions are highly sensitive to the temperature.

From Figure 4.17, it can be seen that, corrected temperature profile decreased the mole fraction predictions of phenanthrene especially HAB greater than 2 mm. The model predictions for phenanthrene were closer to the experimental data with the usage of the corrected temperature profile.

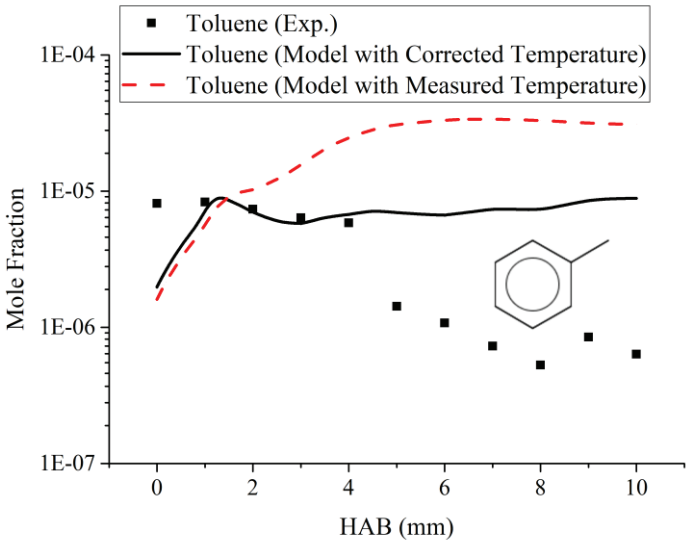

Figure 4.16. Effect of temperature profile to toluene mole fraction

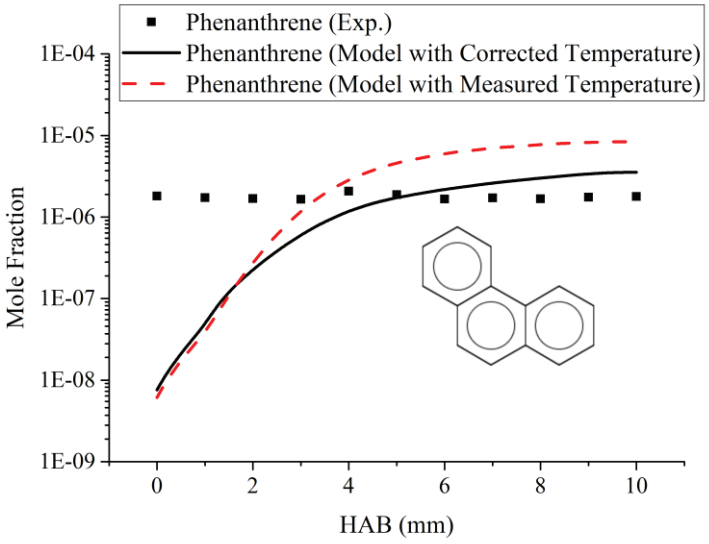

Figure 4.17. Effect of temperature profile to phenanthrene mole fraction.

The comparison of model predictions of pyrene mole fractions by using corrected and measured temperature profile with the experimental data was shown in Figure 4.18.

As seen from Figure 4.18, the pyrene mole fraction predictions were also decreased by a factor of ~10 when corrected temperature profile was used, However, the decrease at the pyrene mole fraction predictions resulted to an underprediction by a factor of ~3, when we compare it to the experimental data.

As a result of the investigation of the effect of the temperature profile to the model prediction of the flame, it can be said that, for some species the uncertainties in the temperature measurements can have significant impact on mole fraction predictions.

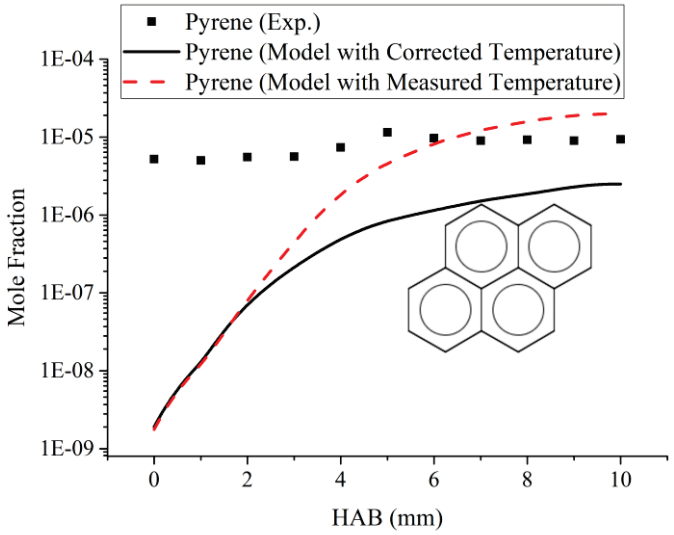

Figure 4.18. Effect of temperature profile to pyrene mole fraction

4.2. Detailed Analysis for Flame

A detailed analysis of the mechanism for the flame conditions (Inal and Senkan 2002) described in Table 3.2 will be discussed in this section. The rate of production analysis will be done for most of the species to find the elementary reactions that generate most flux on the formation of the species. Another analysis, the sensitivity analysis will be done for some species to understand the effect of rate constant parameters on them, by doing sensitivity analysis limiting reactions for the formation or decomposition of species will also be seen. The pathway analysis is capable to show the formation and decomposition pathways over either carbon or hydrogen fluxes. Basically, carbon flux and hydrogen flux pathways are drawn by the software as following the elemental carbon and hydrogen on the reaction sequences respectively. The thickness of the arrows/lines are proportional with formation ratio of the species for the pathway analysis. Thicker

arrows/lines mean that the reaction(s) rates are faster than thinner arrows/lines reaction(s) rates. Each arrow/line involves all reactions that follows the same path.

Before starting the discussion, it was required to mention that, there were possibly higher amount of uncertainty at microprobe sampling which were very close to the burner surface (HAB=0 mm and HAB=1 mm) because of the possible interactions between the burner surface and the microprobe (Inal 1999). It is required to consider those two experimental data-points which were very close to the burner surface less reliable, especially for PAHs.

As seen from Figure 4.19, the master mechanism predicted the species mole fraction profiles of reactants with very low error. In the predictions of master mechanism, fuel completely consumed at lower HAB (~3.5 mm) than the measured profile.

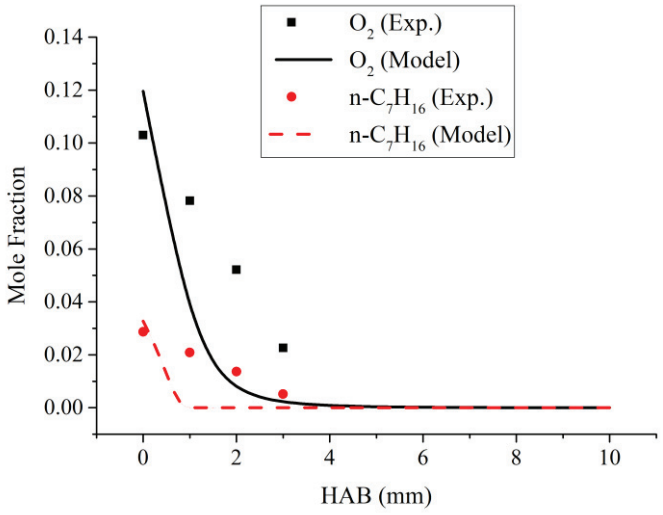

Figure 4.19. Comparison of species profiles of O_2 and n-heptane

As seen from Figure 4.20 all decomposition reactions for n-heptane occurred in HAB range 0 to ~1.3 mm. Hydrogen abstraction reactions by H radical that breaks the C-H bond at the second and third carbon were the most dominant reactions at the decomposition of n-heptane. Hydrogen abstraction reactions by OH radical starts ~0.1 mm earlier than hydrogen abstraction reactions by H radical. This is very reasonable since H radicals form higher HAB on the flame. At ~0.4 mm HAB, third body reactions that form C_4 and C_3 alkyls start. Since all decomposition reactions were in competition at HAB~0.8 mm the closest grid point (HAB=0.8125 mm) was chosen to make the pathway analysis. The path of carbon and hydrogen could be seen separately by two-pathway

analyses, hydrogen elemental flux and carbon elemental flux. The path of hydrogen is generally affected by the side radical species/reactants. However, for carbon flux the carbon formed generated from n-heptane in this case.

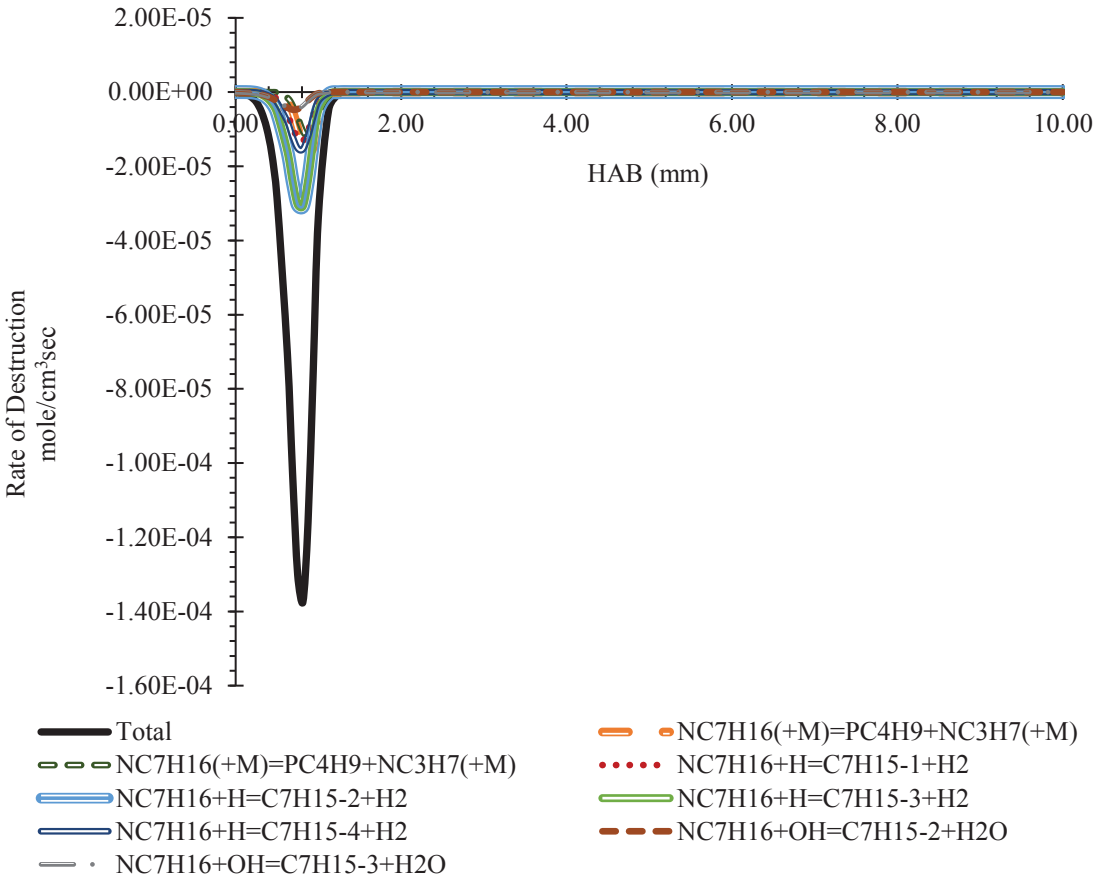

Figure 4.20. Rate of production analysis for n-heptane

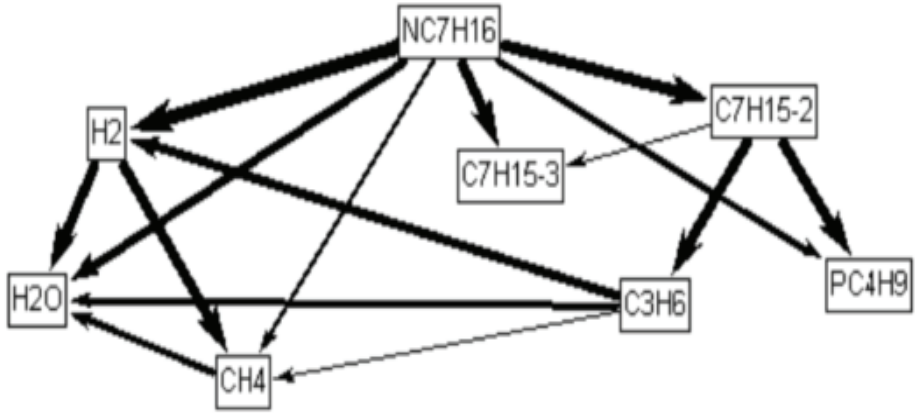

Figure 4.21. Main decomposition pathways of n-heptane at HAB= 0.8125 mm (hydrogen flux)

From the decomposition pathways of n- heptane it can be understood that, the hydrogen abstraction reactions by H were resulted to most of the H2 formation (Figure 4.22). Hydrogen was also formed from the hydrogen abstraction reactions from C3H6. Major consumption pathways for hydrogen were OH+H2=H+H2O and $H_2+CH_3=H_2O+CH_4$ reactions.

Hydrogen abstraction reactions from n-heptane by OH radical was the main reason for the H_2O formation at HAB=0.8125 mm. Since the decomposition rates of 3-heptyl were slower compared to 2-heptyl no decomposition pathway for 3-heptyl (C7H15-3) were shown in Figure 4.22. 3-heptyl starts deforming at higher HAB which was close to the 1 mm according to the computational grid, since 3-heptyl is more stable than 2-heptyl.

The formation of 3-heptyl (C7H15-3) and 2-heptyl (C7H15-2) from n-heptane were almost the same since thickness of the lines were very similar (Figure 4.22). After that 2-heptyl broke down to propene (C3H6) and 1-butyl (PC4H9). The decomposition path for 3-heptyl was not available in the graph since the decomposition rates of 3-heptyl were very low at HAB=0.8125 mm. Additionally, 1-butyl (PC4H9). and ethyl (C2H5) were directly formed from n-heptane by third body reaction.

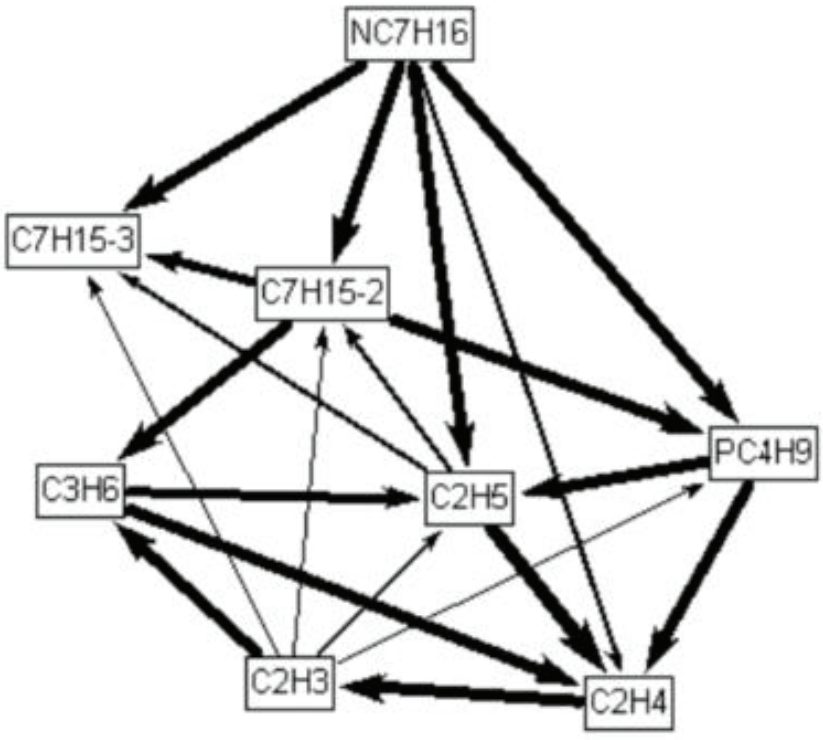

Figure 4.22. Main decomposition pathways of n-heptane at HAB= 0.8125 mm (carbon flux)

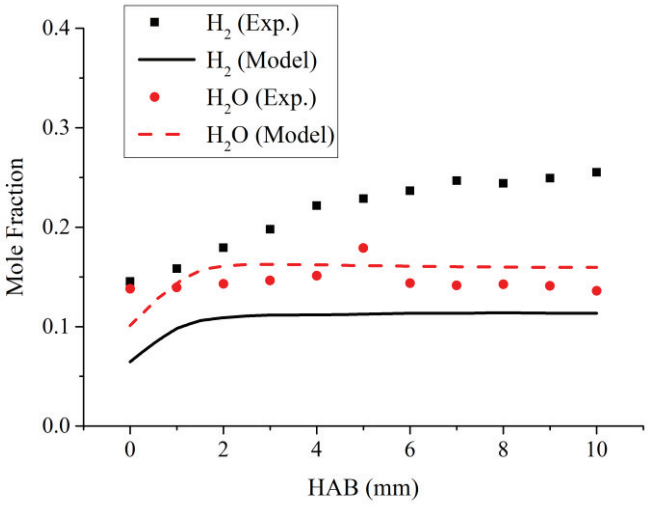

Figure 4.23. Comparison of species profiles of H_2 and H_2O.

The predicted H_2O mole fraction profile was matching with the experimental mole fraction profile (Figure 4.23.). However, the H_2 profile was underestimated by a factor of about 2. For H_2 predictions some of the error might come from the experimental GC/TCD analysis since the retention time of H_2 was very low compared to other species. Additionally, the uncertainties of kinetic and thermodynamic properties in the model could be the possible reasons for the deviations between model predictions and experimental data.

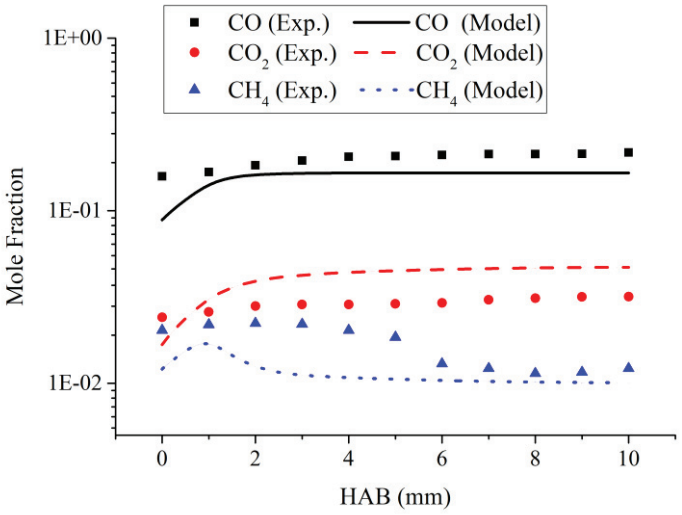

Figure 4.24. Comparison of species profiles of CO and CO_2 and CH_4.

There was a good agreement between model predictions and experimental data for all C_1 (CO, CO_2, CH_4) species (Figure 4.24). For CO_2 the difference between model

predictions and the experimental data was less than a factor of 2. Methane mole fractions was underestimated by the model for 1 mm < HAB < 5 mm.

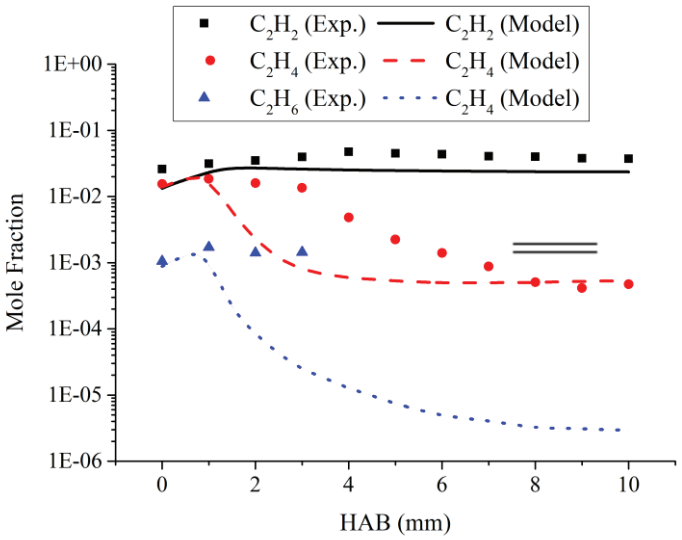

Figure 4.25. Comparison of species profiles of C_2H_2, C_2H_4 and C_2H_6.

The model estimated the C_2 species were very close to the measured mole fraction profiles. Since C_2H_2 is considered as one of the precursor species for first aromatic ring formation and PAH growth (Richter and Howard 2000), rate of production analysis was carried out for acetylene across the flame.

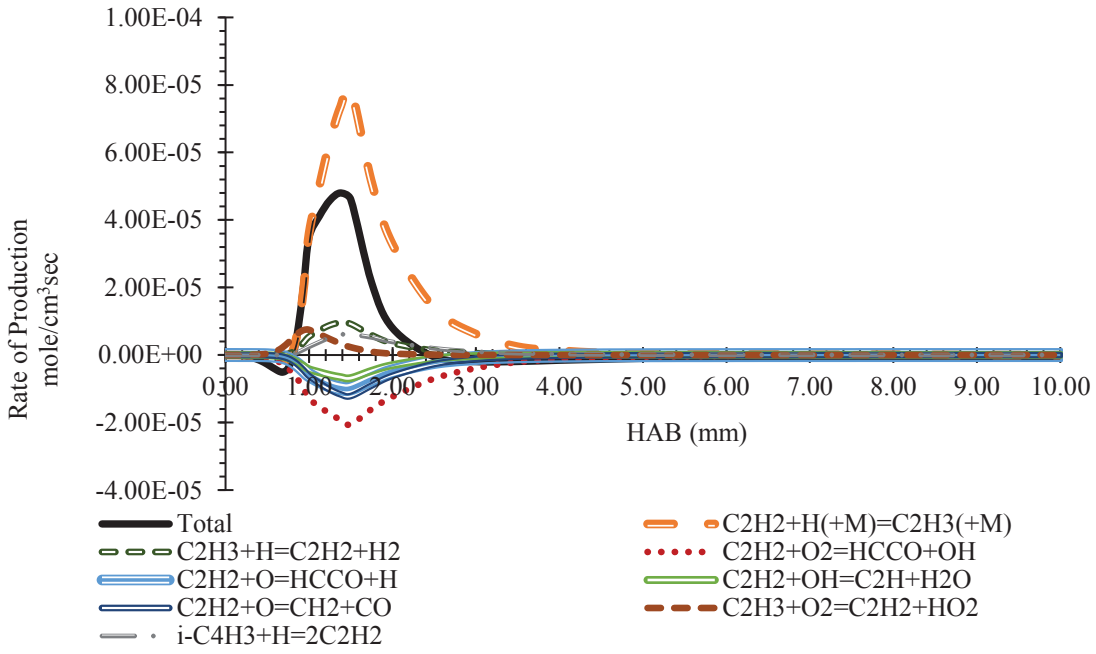

Figure 4.26. Rate of production analysis for C_2H_2 across the flame.

Acetylene was mostly formed by reverse reaction of the C2H2+H+M=C2H3+M (Figure 4.26). Major decomposition pathway for acetylene was the reaction with O_2 which forms formaldehyde (HCCO) and OH radical. Decomposition of acetylene by O and by OH were also major paths. Decomposition of vinyl radical by O_2 at lower HAB and decomposition of vinyl at slightly higher HAB were also resulted in acetylene formation. Since most of the reactions were in competition at HAB~1.5 mm the pathway analysis was performed at that distance.

Most of the acetylene produced HCCO (formaldehyde) by the reactions with O_2 and O (Figure 4.27). CH2 and CO were the other products that are formed from acetylene reacting with O. Water was also formed from acetylene by collision with OH radical at HAB=1.5 mm. Formation pathways for acetylene can be seen from Figure 4.28. Acetylene was mainly formed from vinyl radical, C_2H_3, resulting from the reverse third body reaction, C2H2+H(+M)=C2H3 and the hydrogen abstraction reaction C2H3+H=C2H2+H2 (Figure 4.28).

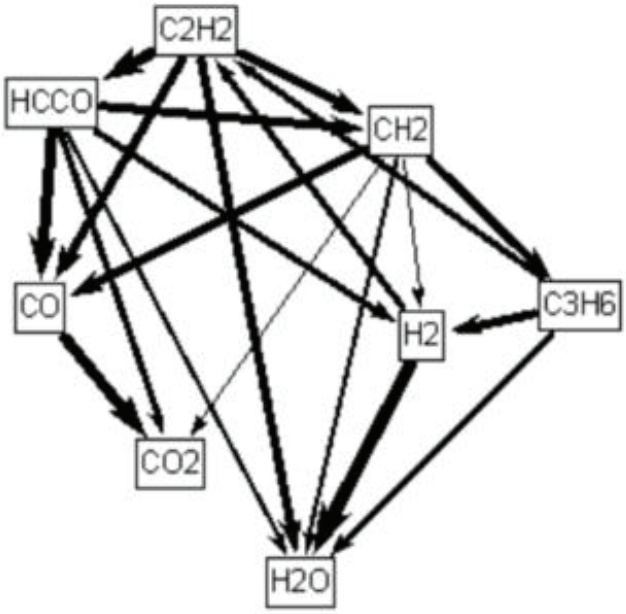

Figure 4.27. Acetylene decomposition pathways at HAB=1.5 mm (both H and C flux)

Third body reaction that forms H_2 and C_2H_2 from C_2H_4 and collision of vinyl radical with methyl radical were also resulted in acetylene formation. Other two reaction paths resulted in acetylene formation involving C2H6 (ethane) and C2H5 (ethyl) were ~10^3 times slower than C2H3 (vinyl) and CH3 (methyl) paths. Sensitivity analysis for acetylene was shown in Appendix A (Figure A. 1.).

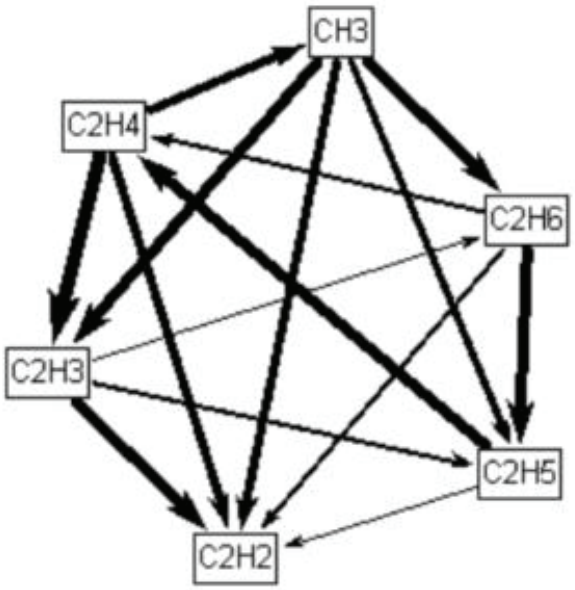

Figure 4.28. Formation pathways of acetylene (C2H2) at HAB=1.5 mm

The experimental data (Inal and Senkan 2002) and model predictions for C_3 species mole fractions were shown in Figure 4.29.

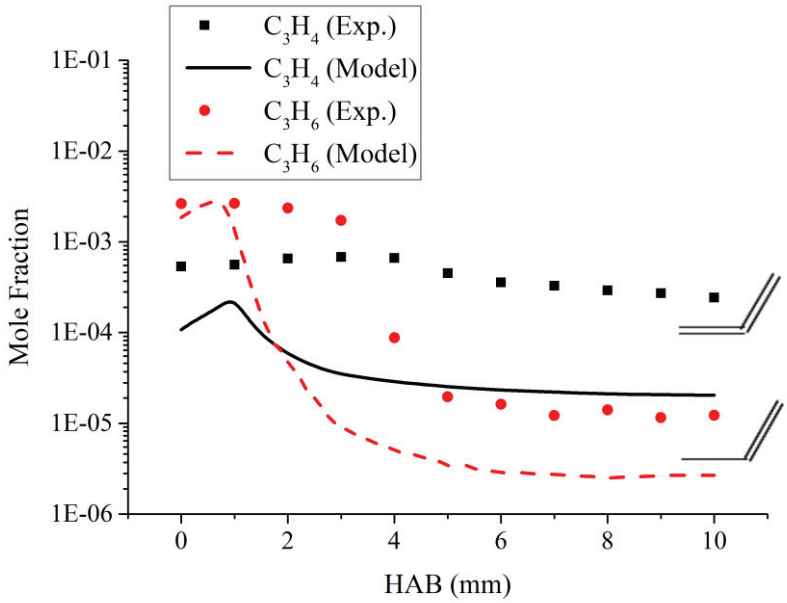

Figure 4.29. Comparison of species profiles of C_3H_4 and C_3H_6

Except from the shift to the burner surface the mechanism caught the propene (C_3H_6) mole fraction profile (Figure 4.29). However, propadiene (C_3H_4) was underestimated by the master mechanism by a factor of 10. Since odd carbon number

species propadiene was considered as precursor for the formation of first aromatic ring, rate of production analysis was done for this species.

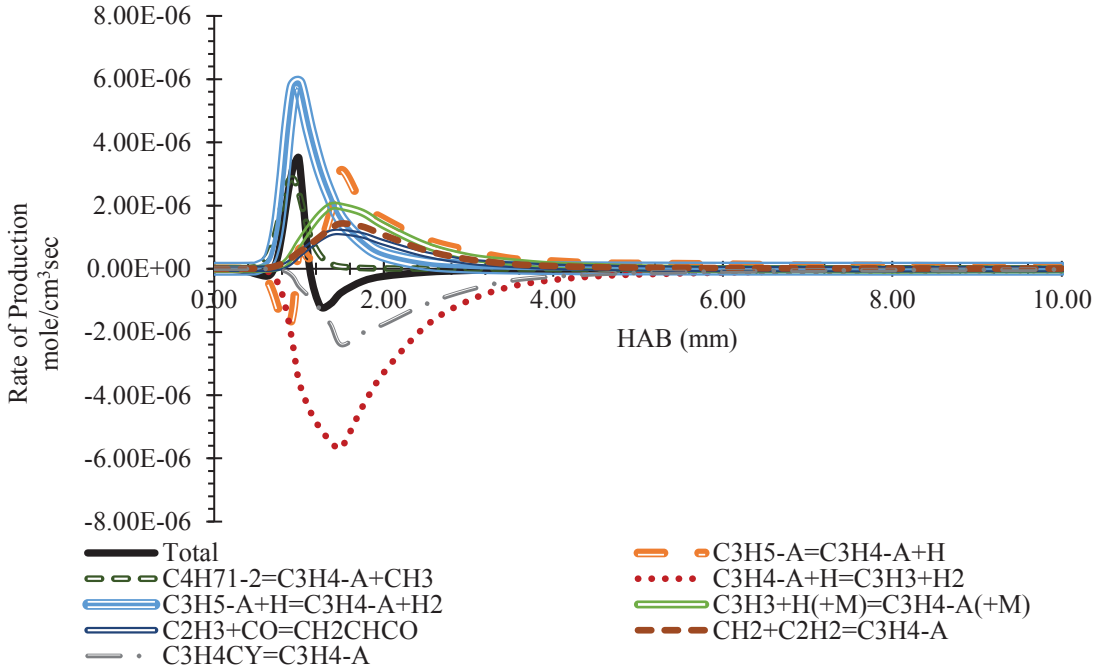

Figure 4.30. Rate of production analysis for propadiene across the flame

The most important pathway that resulted in propadiene formation was hydrogen abstraction from allyl radical, at the lower heights on the burner surface (~0.7 mm) -but-2yl-1ene (C4H71-2) decomposition was resulted in propadiene and a methyl radical (Figure 4.30). The fastest reactions at the destruction of allene were C3H4-A+H=C3H3+H2, C3H4CY=C3H4-A (C3H4CY is refereed to cyclopropane). At the lower points on the burner (<0.8 mm), reverse reaction of C3H5-A=C3H4-A+H were faster than the forward reaction. At the higher HAB the forward reaction becomes one of the effective reactions on the formation of propadiene. In general, most of the C3H4-A was formed at HAB~0.9 mm and decomposed at HAB~1.4 mm. The formation pathway for propadiene was shown at the closest grid point to HAB ~0.9 mm and decomposition was shown at ~1.4 mm. The most of the allene (propadiene) was formed from allyl radical (C3H5-A) by hydrogen abstraction reaction (Figure 4.31). Hydrogen removal from propene (C3H6=C3H4-A+H2) was another pathway that resulted in allene formation. Collison of 1-propyl (NC3H7) with allyl radical also resulted in allene formation with ~10^4 times slower than the major pathway at HAB=0.9375 mm.

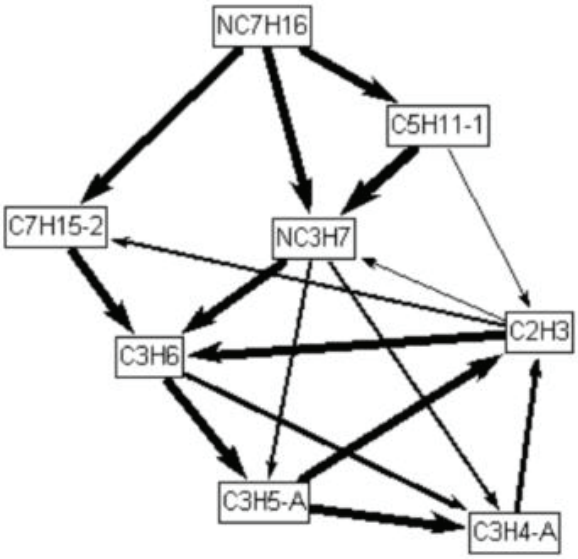

Figure 4.31. Formation pathways of propadiene at HAB=0.9375 mm (both H and C flux)

The difference between measured and estimated C_4H_2 and C_4H_4 mole fractions were less than a factor of 10 (Figure 4.32.). However, the mechanism was capable to compute the trend. The estimated 1,3-butadiene (C_4H_6) profile coincides with the experimental data.

Since C_4H_4 is considered as a major precursor for benzene, and larger aromatic hydrocarbons, the rate of production analysis across the flame (Figure 4.33) was done for vinylacetylene (C4H4).

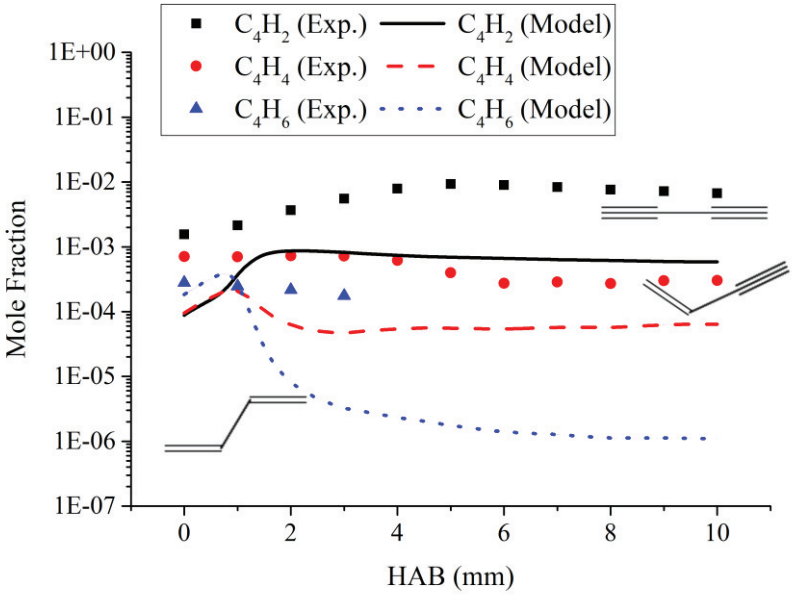

Figure 4.32. Comparison of species profiles C_4H_2, C_4H_4 and C_4H_6

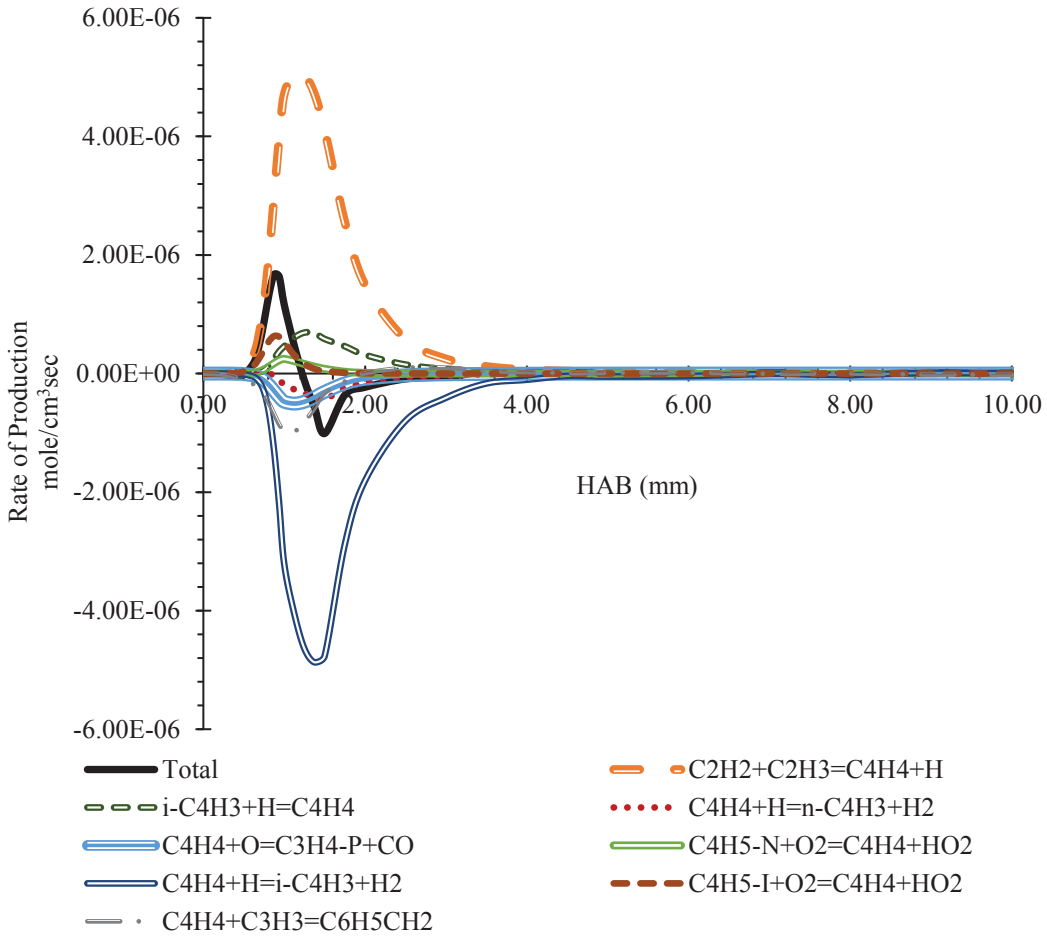

Figure 4.33. Rate of production analysis for vinylacetylene across the flame

Vinylacetylene was generally formed at HAB~1.5 mm by the reaction between C2H2 (acetylene) and C2H3 (vinyl radical) (Figure 4.33). The main destruction of C_4H_4 resulted from hydrogen abstraction reaction from vinylacetylene which forms but1ene,2yl,3yne (i-C4H3) and hydrogen. Another hydrogen abstraction reaction that forms but1ene,1yl,3yne (n-C4H3) was a slower destruction path for vinylacetylene. The reaction between propargyl radical (C3H3) and vinylacetylene was also responsible for the consumption of vinylacetylene. The total rate of production of vinyl acetylene was positive up to ~1.2 mm HAB then the total rate of production became negative. The pathway analysis was done at HAB ~1 mm and ~1.5 mm to see the competition between production and destruction reactions, respectively.

Most of the vinylacetylene was formed from vinyl radical by the combination reaction of acetylene and vinyl radical as seen from Figure 4.34. Additionally, ethylene (C2H4) was another reactant that forms vinyl acetylene by combination reaction of ethylene and C2H (ethyne).

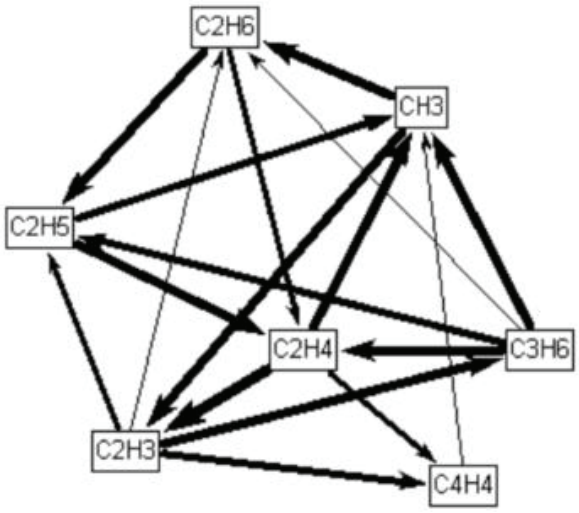

Figure 4.34. Simplified formation pathways of Vinylacetylene at HAB=1 mm (both H and C flux)

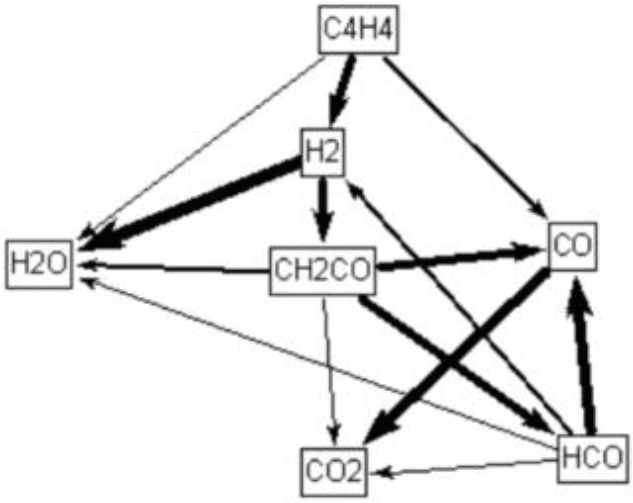

Figure 4.35. Simplified decomposition pathways of Vinylacetylene at HAB=1.5 mm (both H and C flux)

The hydrogen abstraction reactions between H radical and vinyl acetylene which forms H2 (hydrogen) was the most important path for decomposition as seen in Figure 4.35 at HAB=1.5 mm. Other paths for vinyl acetylene decomposition were bimolecular collision of C4H4 with O and OH radical which forms CO and H2O, respectively.

Both benzene and Phenylacetylene mole fraction profiles were over-estimated by the master mechanism for HAB > 4 mm (Figure 4.36.) Benzene was considered as first aromatic rings in non-aromatic hydrocarbon flames (Richter and Howard 2000). So that rate of production analysis for benzene was carried out across the flame.

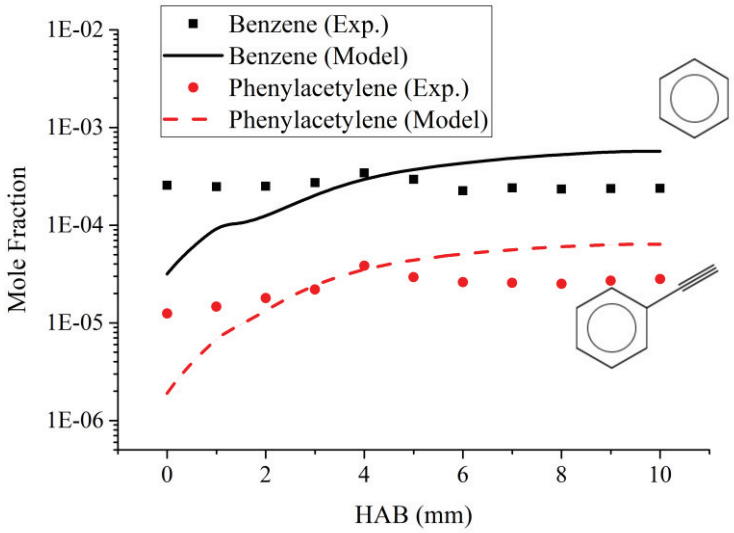

Figure 4.36. Comparison of species profiles of benzene and phenylacetylene

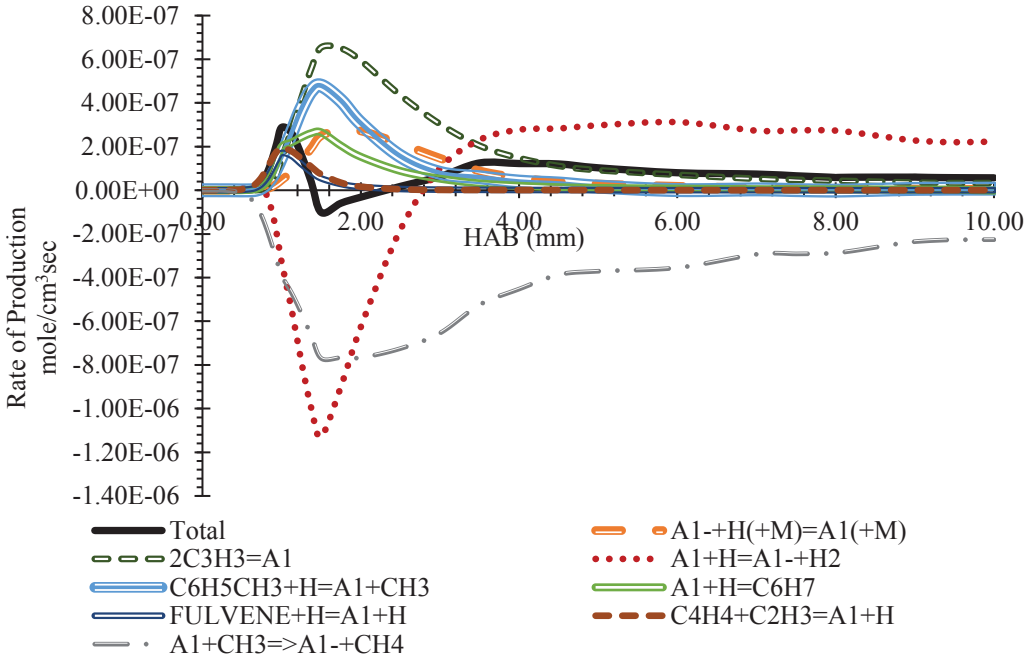

Figure 4.37. Rate of production analysis for benzene (A1) across the flame

As seen from Figure 4.37 the total rate of production of benzene was positive for HAB lower than 1.6 mm. For 1.6 mm <HAB< 2.4 mm benzene decomposition reactions were faster than the production reactions. Then the total rate of production of benzene became positive again. The most effective reactions for benzene destruction and formation seems to be hydrogen abstraction reaction from benzene. Combination of propargyl (C3H3) reactions also resulted in benzene formation especially at HAB ~2 mm.

The forward reaction between toluene and H (C6H5CH3+H=A1+CH3) also resulted to benzene formation. For the formation of benzene, the pathway analysis was done at two HAB ~1.2 mm and ~4 mm to see different formation pathways that depend on height above the burner.

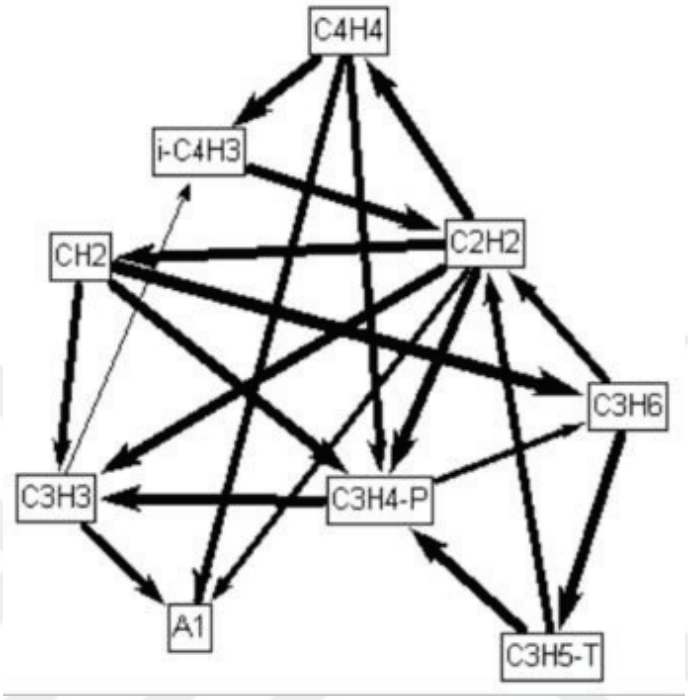

Figure 4.38. Simplified formation pathways of benzene (A1) at HAB=1.25 mm (both H and C flux)

The recombination reaction between two propargyl radicals (2C3H3=A1) was produced most of the benzene (Figure 4.38.). Additionally, bimolecular reaction between vinylacetylene and vinyl radical (C4H4+C2H3=A1+H) also resulted to comparable benzene formation. Direct paths from acetylene to benzene were quite slow compared to previously mentioned paths. However, acetylene was the main reactant that forms vinylacetylene and propargyl radical so that it has a significant precursor for benzene formation. Different from Seidel et al. (2015) who were studied on low pressure n-heptane flame fulvene pathways that forms benzene was found less important than the vinylacetylene and propargyl pathways. Reactions between C_4H_x and C_2H_y species were found as an important pathway that forms benzene in atmospheric n-heptane flames and proposed by various studies (Raj et al. 2012, Wang et al. 2015).

The recombination reaction of propargyl radical was also the main benzene formation reaction at HAB=4.0 mm similar with HAB=1.25 mm (Figure 4.39.). However,

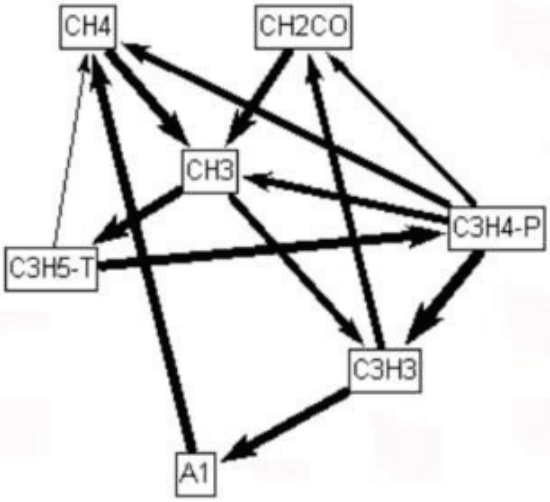

Figure 4.39. Simplified formation pathways of benzene (A1) at HAB=4.00 mm (C flux)

the vinylacetylene path was ~100 times slower when comparing with HAB=1.25 mm (Figure 4.38.). Additionally, direct path from acetylene was also slower compared with the HAB=1.25 mm. These results can be explained by the number of free radicals on the flame which was higher at 0.125 mm HAB than 4 mm HAB. Additional pathway for benzene at HAB=4.0 mm was drawn at Figure 4.40 for hydrogen flux to see the path of hydrogen that forms benzene.

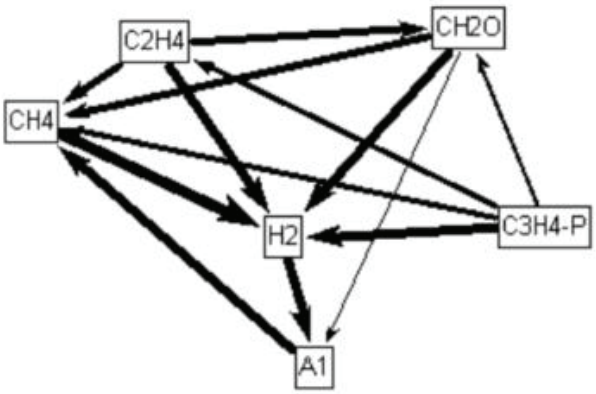

Figure 4.40. Simplified formation pathways of benzene (A1) at HAB=4.00 mm (H flux

As seen from Figure 4.40. for benzene formation most of the hydrogen flux was from molecular hydrogen by the reverse of the hydrogen abstraction reaction (A1+H=A1-+H2). Some hydrogen was split from benzene by collision with methyl radical (A1+CH3=A1-+CH4) and formed methane at HAB = 4.0 mm.

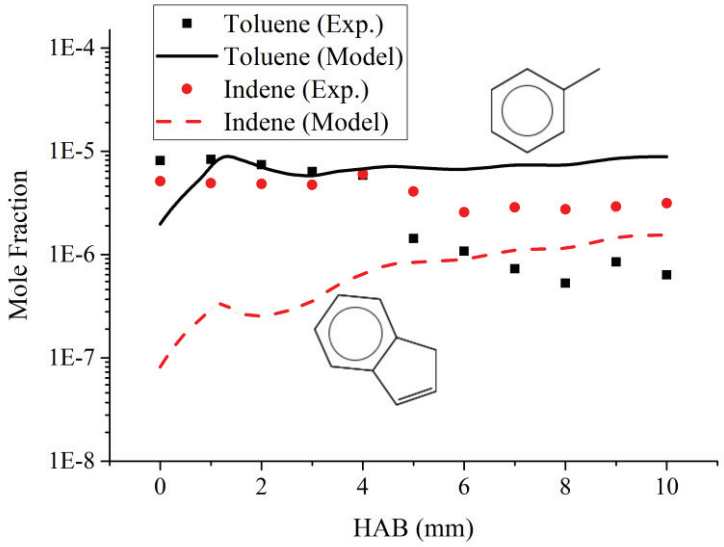

Figure 4.41. Comparison of species profiles of indene and toluene

The predicted toluene and indene mole fraction profiles together with experimental data could be seen in Figure 4.41. Toluene mole fractions were predicted by the master mechanism with low error for HAB < 4 mm. For HAB > 5 mm the model overpredicted the toluene mole fractions by a factor of about 10 (Figure 4.41). Indene mole fractions were underpredicted by a factor of around 3 on height above the burner greater than 5 mm. For indene difference between model predictions and experimental measurements decreased when the height above the burner increased (Figure 4.41.).

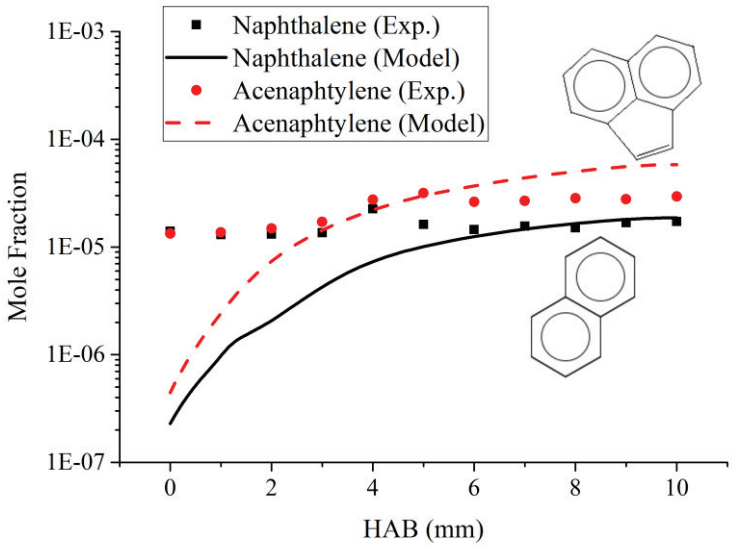

Figure 4.42. Comparison of species profiles of naphthalene and acenaphthylene

The master mechanism predicted the acenaphthylene and naphthalene mole fraction profiles with low error when comparing with the measured species mole fraction profiles (Figure 4.42). As a reference for two ring aromatic hydrocarbon, the rate of production analysis and pathway analysis were done for naphthalene (A2). As seen from Figure 4.43 the total rate of formation profile of naphthalene was very similar with total rate of production of benzene (Figure 4.37).

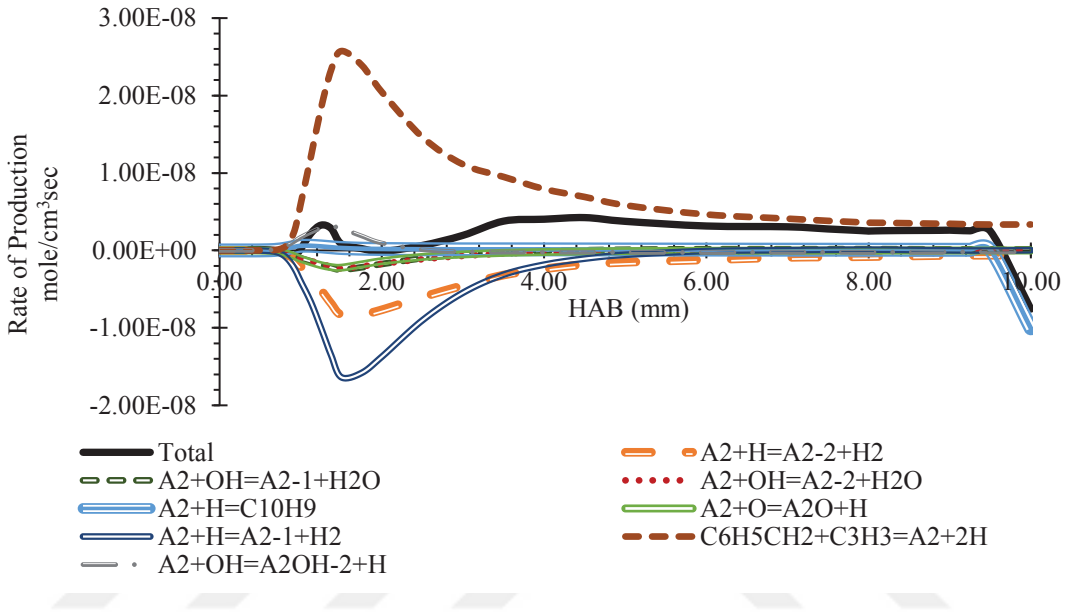

Figure 4.43. Rate of production analysis for naphthalene (A2) across the flame

For naphthalene, most productive reactions seem to be the reaction between benzyl radical and propargyl radical (C6H5CH2+C3H3=A2+2H) (Figure 4.43). For the destruction of the naphthalene hydrogen abstraction reactions that forms naphth-2-yl (A2-2) and naphth-1-yl (A2-1) (A2+H=A2-2+H2 and A2+H=A2-1+H2) were important.

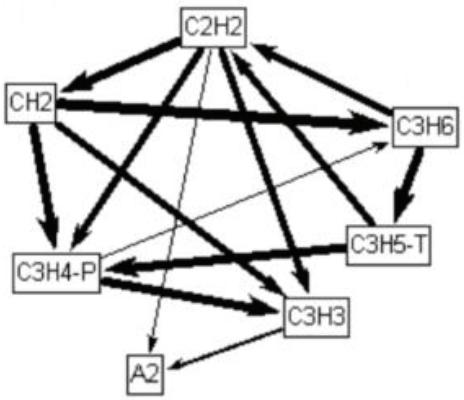

Figure 4.44. Simplified formation pathways of naphthalene (A2) at HAB=1.25 mm (both H and C flux)

For the formation of naphthalene two formation pathways were drawn which corresponds to ~1.2 mm and 4 mm HAB. As seen from Figure 4.44. the reaction between benzyl and propargyl was the most important reaction for the formation of naphthalene formation at HAB= 1.25 mm. The acetylene pathway for naphthalene formation was about 1/10 of the propargyl path. The formation path that involves cyclopentadienyl radical with the reaction (2C5H5=A2+2H) was found as around 100 times slower than the benzyl path which was a contradictive result to the study of Seidel et al. (2015). However, the difference between the flame pressures could be the reasons of different paths that resulted in naphthalene formation.

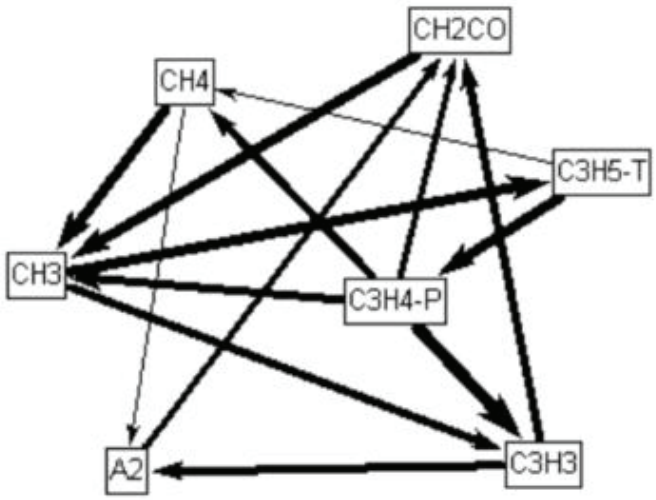

Figure 4.45. Simplified formation pathways of naphthalene (A2) at HAB=4.0 mm (both H and C flux)

Similar with HAB = 1.25 mm, the most important reaction for the formation of naphthalene was found as (C6H5CH2+C3H3=A2+2H) at HAB = 4 mm. Other paths that resulting with naphthalene formation were ~10 times slower than the one involving propargyl and benzyl. The contribution of cyclopentadienyl was around 10^{-3} of propargyl.

As seen from the master mechanism was caught both phenanthrene and anthracene species profile with an error less than a factor of 3 especially at the higher distance above the burner surface (Figure 4.46). As a representative for 3 ring PAH, rate of production analysis was done for phenanthrene across the flame.

As seen from Figure 4.47 the rate of production profiles of phenanthrene (A3) was highly different than smaller aromatic species (Figure 4.37, Figure 4.43). The most of the phenanthrene formed was from the reaction between cyclopentadienyl radical and indenyl

radical (C9H7+C5H5=A4+2H). Biphenyl radical (P2-) and phenyl acetylene (A1C2H) were the other reactants that forms phenanthrene. The decomposition of phenanthrene results from hydrogen abstraction reactions that forms various phenanthryl isomers. The pathway analysis was done at the HAB = 4.0 mm which corresponds to the peak of total phenanthrene ROP.

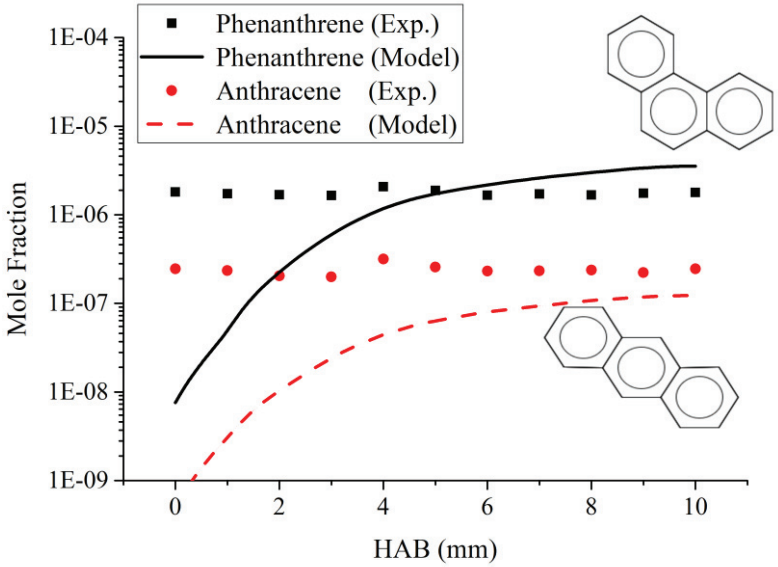

Figure 4.46. Comparison of species profiles of phenanthrene and anthracene

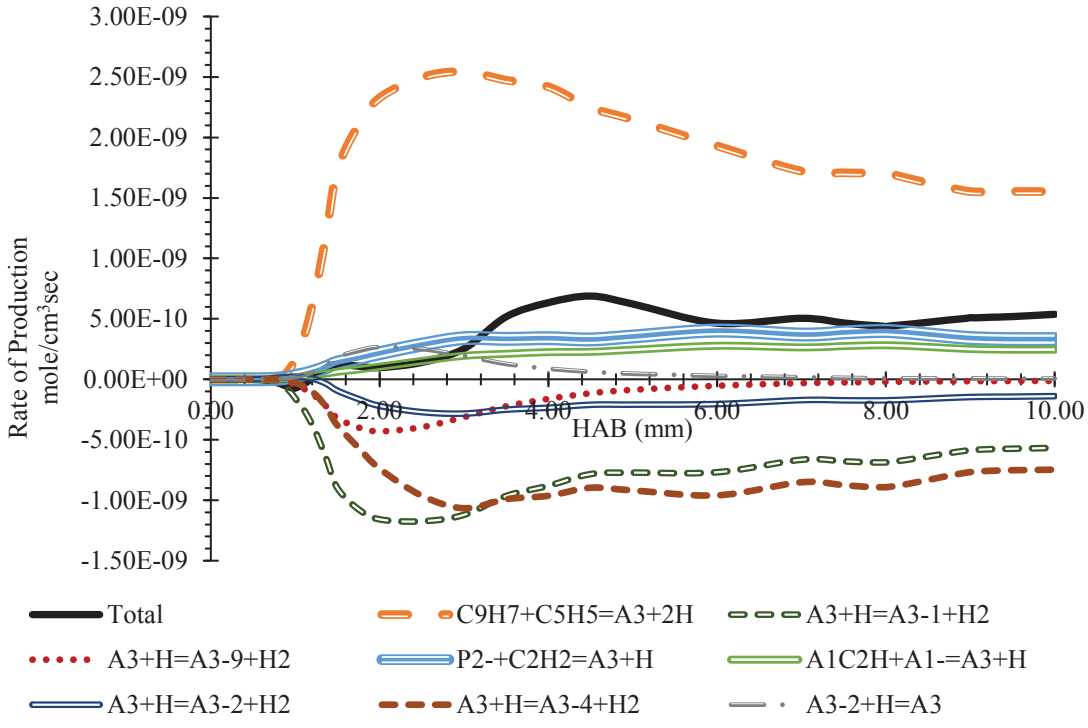

Figure 4.47. Rate of production analysis for phenanthrene (A3) across the flame

The most of the phenanthrene was formed from cyclopentadienyl radical (C5H5) at HAB = 4.0 mm according to model (Figure 4.48). The path that involves phenyl (A1-) was about 10 times slower than C_5 path. Although, it was not shown in Figure 4.48, other paths that involves phenylacetylene (A1C2H+A1-=A3+H) and biphenyl radical (P2-+C2H2=A3+H) were had comparable ROP with phenyl (A1-) path. For phenanthrene formation, reactions involving vinylacetylene and acenaphthylene were found important in n-heptane flames (Wang et al. 2015). However, those paths were not included in this version of the master mechanism.

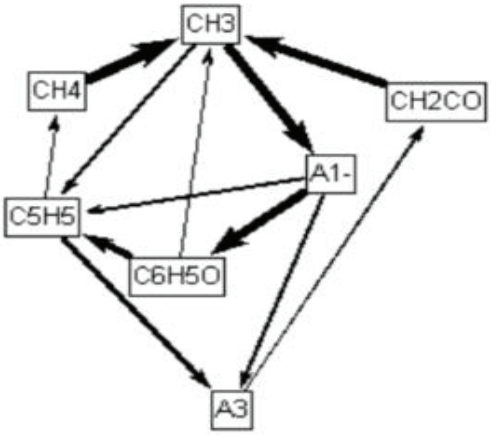

Figure 4.48. Simplified formation pathways of phenanthrene (A3) at HAB=4.0 mm (both H and C flux)

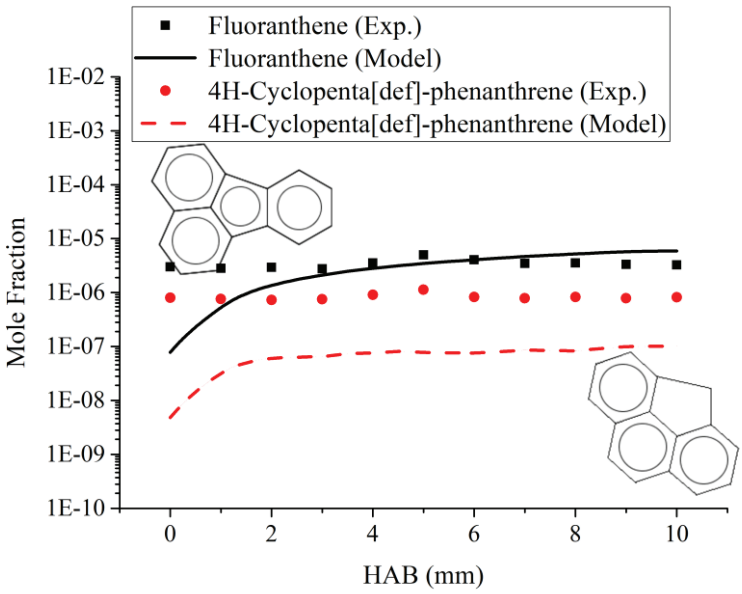

Figure 4.49. Comparison of species profiles of fluoranthene and 4H-Cyclopenta[def]-phenanthrene

The difference between master mechanism predictions of fluoranthene and experimental data was less than a factor of about 1.5 (Figure 4.49).

However, 4H-Cyclopent[def]-phenanthrene mole fractions were underestimated by the master mechanism by a factor of about 10. Some difference between measured and estimated mole fractions of 4H-Cyclopent[def]-phenanthrene could be caused from experimental uncertainties. However, it was certain that additional reactions were required to explain 4H-Cyclopent[def]-phenanthrene formation kinetics.

As seen from Figure 4.50, the difference between measured and estimated mole fraction was less than a factor of 5 for pyrene. However, aceanthrylene was overestimated with a factor of about 10 for HAB > 6 mm. The rate of production analysis was done for pyrene as a representation of the formation of 4 membered PAHs.

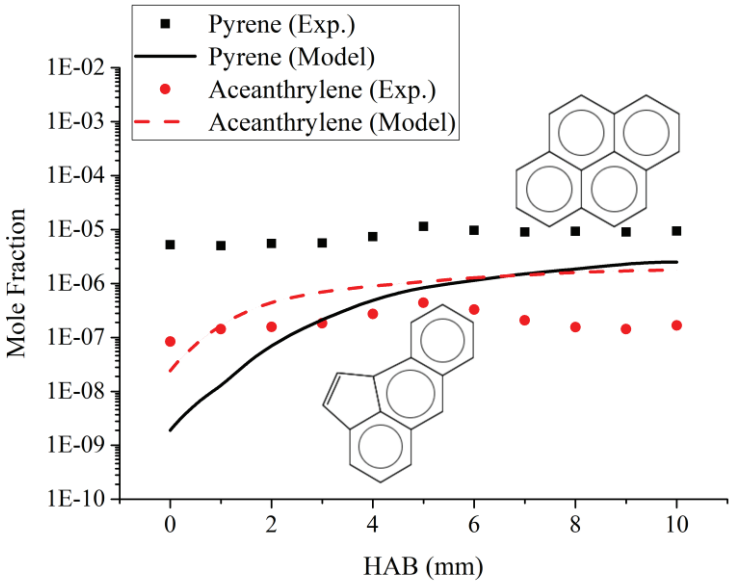

Figure 4.50. Comparison of species profiles of pyrene and aceanthrylene

The important reactions for the formation/decomposition of pyrene involved the reaction of and free radicals (OH, H) except 2C9H7=>A4+C2H2+H. (Figure 4.51).

The Pathway analysis was done for pyrene at HAB = 4.0 mm. Pyrene was mostly produced by the recombination reaction of indenyl radical (C9H7) (Figure 4.52). The path that involves HACA growth, (A3-1+C2H2=A4+H) and (A3-4+C2H2=A4+H) was around ½ of the C9H7 path. Several paths that are important for the formation of pyrene seem to be missing in the master mechanism. Cyclopenta[cd]pyrene mole fraction profile was estimated by the mechanism with an error that less than a factor of about 5 (Figure 4.53). However, the benzo[ghi]fluoranthene mole fractions were under-estimated by the

master mechanism with an about ~50 times lower than measured mole fractions. It was definite that, more reactions are required to clarify the formation paths of benzo[ghi]fluoranthene.

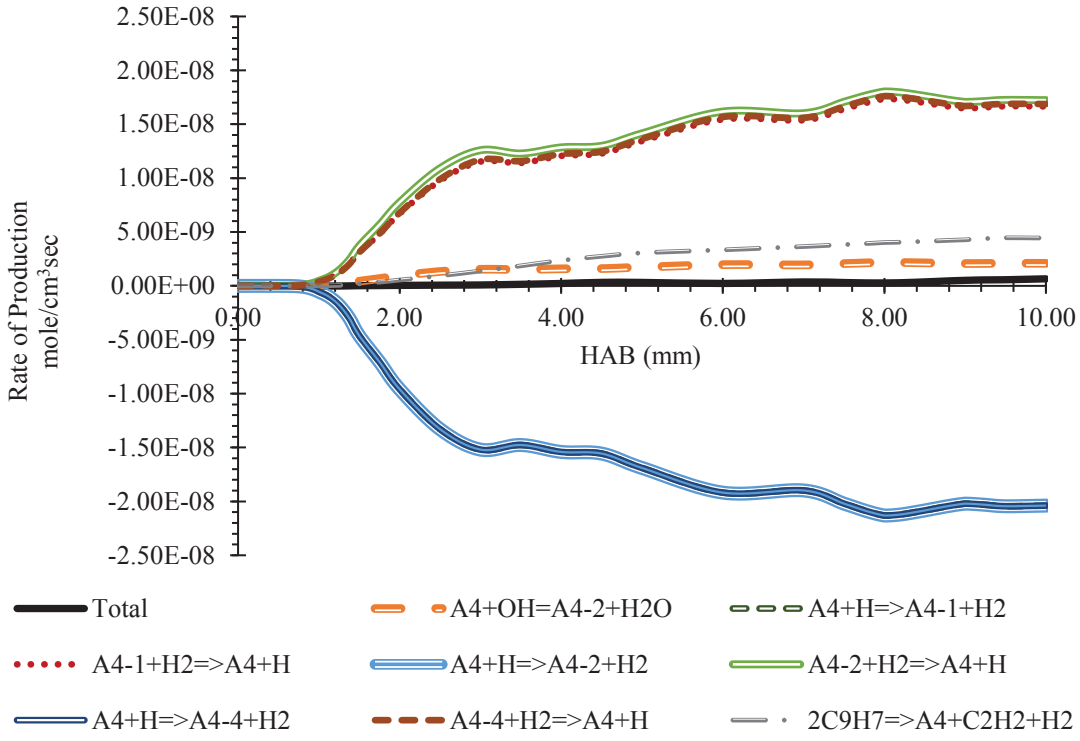

Figure 4.51. Rate of production analysis for phenanthrene (A4) across the flame

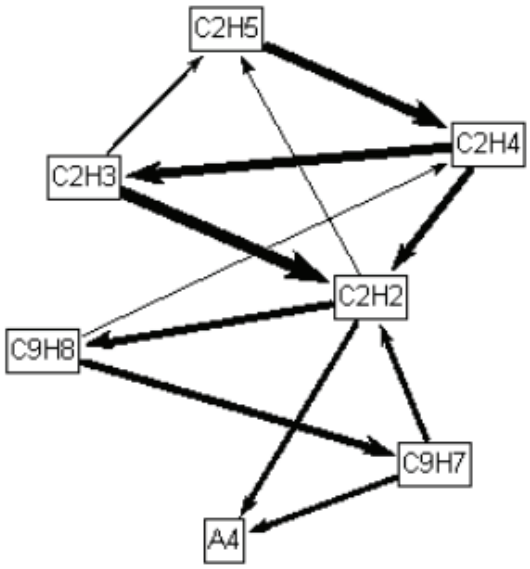

Figure 4.52. Simplified formation pathways of phenanthrene (A4) at HAB=4.0 mm (both H and C flux)

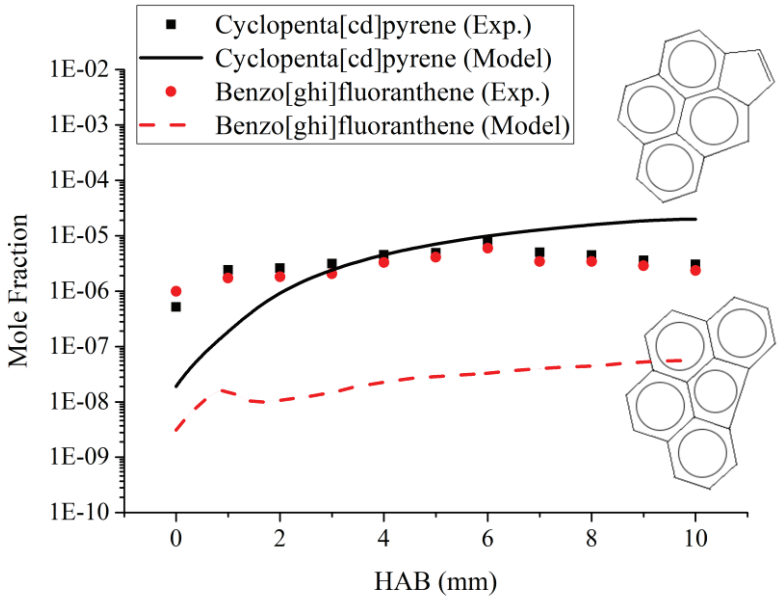

Figure 4.53. Comparison of species mole fraction profiles of cyclopenta[cd]pyrene and benzo[ghi]fluoranthene

There were also some species that detected in the GC/MS analysis at one or two points on HAB, these species were not quantified because of their low concentrations (Inal 1999). However, the model also predicted the mole fraction profiles of those species (1-butyne, cyclopentadiene, styrene, 1,2-dimetylbenzene, biphenyl, biphenylene, fluorene, and ethylbenzene), (Figure 4.54 - Figure 4.57).

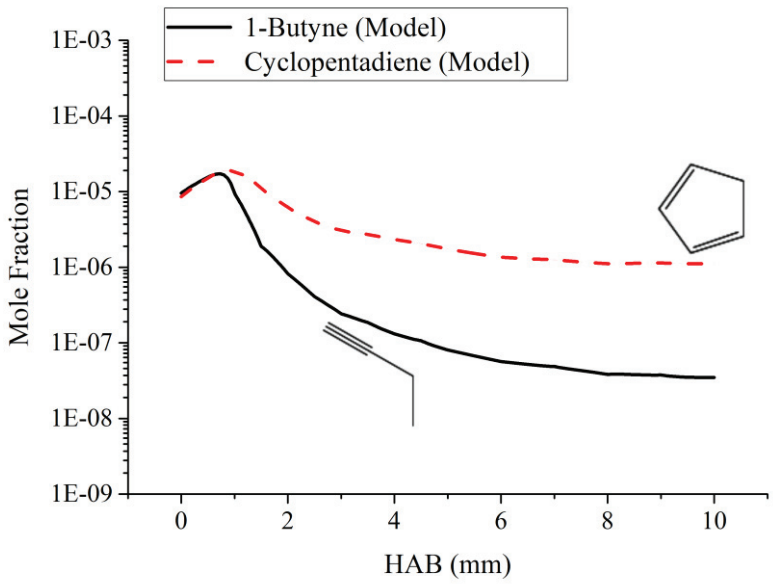

Figure 4.54. Mole fraction profiles of cyclopentadiene and 1-butyne

As seen from Figure 4.54, the maximum mole fraction for cyclopentadiene and 1-butyne were at HAB ~1 mm. Possible decay of cyclopentadiene at the sampling line might cause to missing experimental points. For the 1-butyne the predicted mole fractions were very low except for HAB ~1 mm which could cause quantification problems.

Similar with 1-butyne and cyclopentadiene, the maximum mole fractions of styrene and 1,2-dimethylbenzene were at HAB of ~ 1 mm, in which sampling with microprobe was a problem since it was very close to the burner surface (Figure 4.55).

The predicted mole fractions of biphenylene were very low ~ 10^{-9} (Figure 4.56). It was improbable to see the maximum mole fraction of biphenylene at the burner surface because most of the n-heptane were not decomposed yet. Since the predicted mol fractions were very low, it can be said that for the n-heptane flame, probability of formation of biphenylene was lower than other PAHs.

The mole fraction profile of biphenyl showed an increasing trend and it reach about 10^{-6} level at HAB = 10 mm (Figure 4.56).

The maximum mole fraction of ethylbenzene was at HAB ~ 1 mm. However, for the rest of the HAB, concentrations of ethylbenzene were very low, thus, due to the insufficient experimental detection limits, it could not be tabulated. The model predicted the maximum mole fraction of fluorene as ~10^{-7} levels for the HAB greater than ~ 3 mm (Figure 4.57).

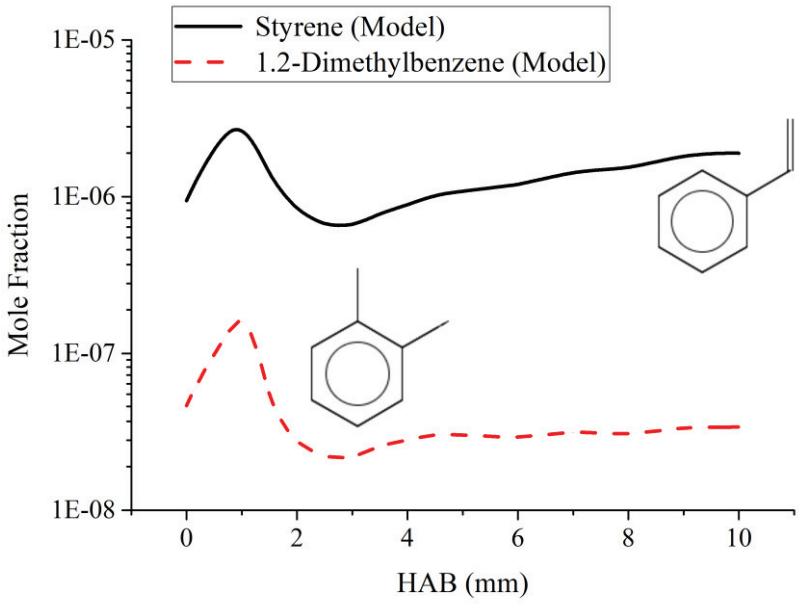

Figure 4.55. Mole fraction profiles of styrene and 1,2 dimethylbenzene

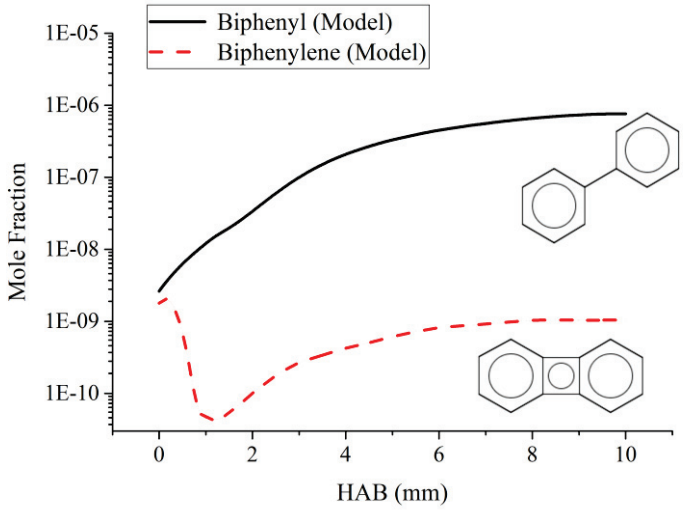

Figure 4.56. Mole fraction profiles of biphenylene and biphenyl

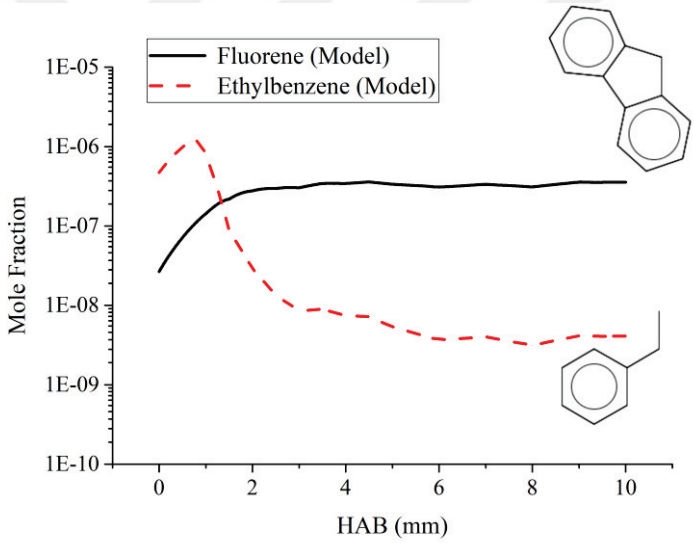

Figure 4.57. Mole fraction profiles of fluorene and ethylbenzene

4.3. Mechanism Reduction

There are several methods suggested in the literature to apply mechanism reduction, such as principal component analysis, directed relation graph method (DRG) (Lu and Law 2005) directed relation graph with error production (DRGEP) (Pepiot-Desjardins and Pitsch 2008), directed relation graph method with path flux analysis

(DRGPFA), and isomer lumping. In this study directed relation graph with error propagation method was used to reduce the master mechanism.

The removal of a species on the production rate of selected species was defined as an immediate error, (r_{AB}) where A is the selected species and B is the removed species. The immediate error calculated by the equation below,

$$r_{AB} \equiv \frac{\sum_{i=1,j} |v_{A,i} \omega_i \delta_{Bi}|}{\sum_{i=1,j} |v_{A,i} \omega_i|} \tag{4.1}$$

$$\delta_{Bi} = \begin{cases} 1, \text{ if the } i^{th} \text{ reaction involves species B} \\ 0, \text{ otherwise} \end{cases} \tag{4.2}$$

where;

i is the reaction number, $v_{A,i}$ is the stoichiometric coefficient of species A in the ith reaction, ω_i is the reaction rate of the ith reaction. Denominator includes the all reactions in the mechanism, however, the numerator just includes the reactions involving species B. If the calculated immediate error is greater than the error-tolerance level which is defined by user, the specie would not eliminated by the algorithm.

Directed relation graph with error propagation (DRGEP) method was used to reduce mechanism. DRGEP is a similar method with the DRG method, however the process that decide which species are required to be removed is different. For DRGEP method R-value is defined for the determination of species that need to be kept in the mechanism. If a species A is kept in the mechanism, the possible species that are from species A through direct and indirect coupling are considered using their "R-value", which is defined as;

$$R_A(B) = \max_S \{r_{ij}\} \tag{4.3}$$

where S is the set of all possible paths leading from species A to species B, and r_{ij} is the chain product of the weights (that is, the immediate error r_{ij}) of the edges along the given path. For the reaction sequence of A→B→C the R value is $r_{AB} \times r_{BC}$. Based on the definition species B must be kept if at least there is a reaction between A and B with a larger R value than the defined threshold.

As the relative tolerance increases, the number of eliminated reactions are also increases. To start mechanism reduction, the relative tolerance of the all minor, major and trace species that experimentally quantified were given as 500 %. By defining the relative

tolerance as a high value, it was possible to see different versions of reduced mechanisms. Reduced mechanisms that have different number of species/reactions could be seen in Figure 4.58. The percentage error was related with the difference between master mechanism and reduced mechanisms mole fraction predictions. There were two sudden increases in the percentage error of n-heptane mole fraction predictions with the increasing threshold value. The second reduced mechanism which corresponds to 0.111 threshold value was chosen as best skeletal mechanism. Even small amounts of further species/reaction removals resulted in high amount of increase in the percentage error (Figure 4.58). The threshold values were related with the removal of the species/reactions. Threshold value of 1 means that removal of all species/reactions. As a result of mechanism reduction, a skeletal mechanism with 1879 reactions and 359 species was achieved. The validations of the skeletal mechanism will be shown in the next section.

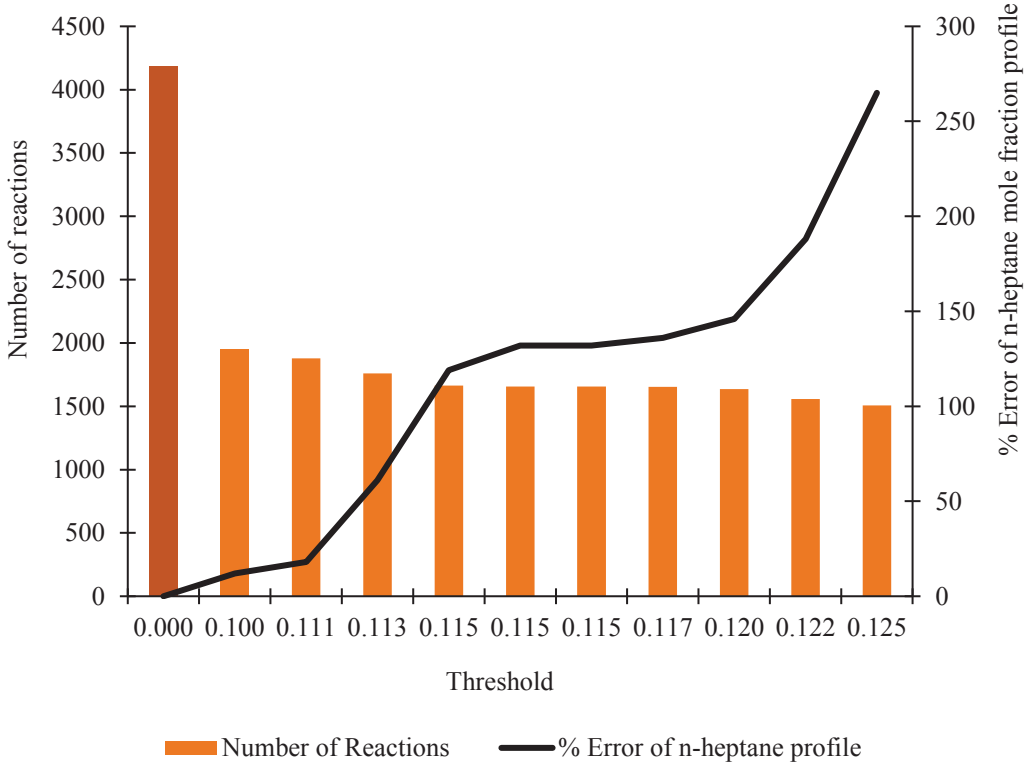

Figure 4.58. Effect of mechanism reduction on n-heptane mole fraction estimations

4.4. Validations of the Skeletal Mechanism

To validate the skeletal mechanism same experimental data used for master mechanism were tested. The experimental conditions for JSR, premixed flame and shock-

tube studies were shown Table 4.1, Table 4.2 and Table 4.3, respectively. As seen from Figure 4.59, reduced (skeletal) mechanism gave similar result with the master mechanism for the n-heptane mole fraction predictions of a JSR reactor. For temperatures between 525 K to 600 K there were a noticeable difference for n-heptane mole fractions. For methane mole fraction in a JSR reactor, the predictions of the master and skeletal mechanism were almost the same (Figure 4.60).

As mentioned before, acetylene mole fractions were overestimated by the master mechanism when comparing with the JSR experimental data. The reduced mechanism gave similar results for the acetylene mole fraction prediction in the JSR (Figure 4.61).

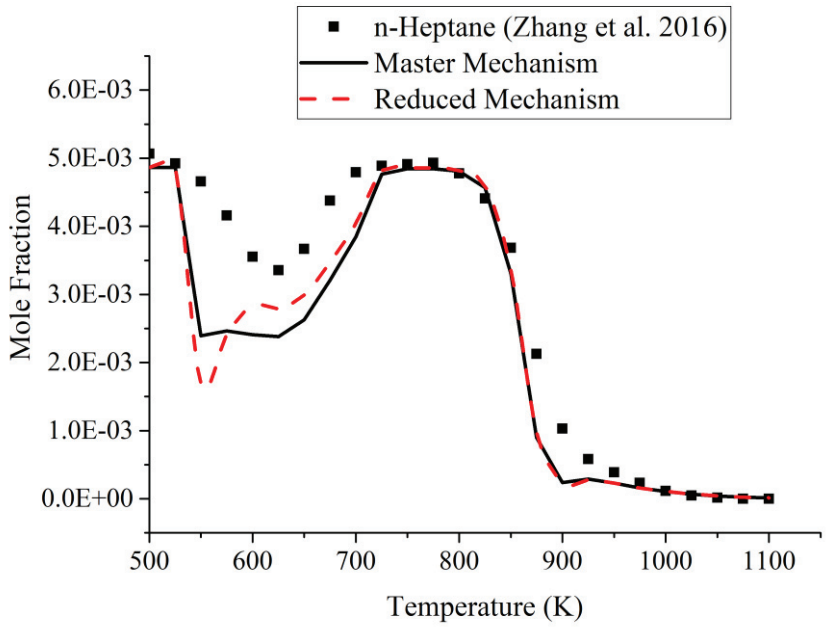

Figure 4.59. Validation of the skeletal mechanism on n-heptane mole fraction with JSR

The reduced mechanism predictions for the benzene mole fractions were very close to the master mechanism results. Both master and reduced mechanisms slightly overestimated the benzene mole fractions comparing with the experimental data of JSR with the equivalence ratio of 2.

Most of the reactions that removed from the master mechanism was probably related with low temperature oxidation pathways of n-heptane. So that there was almost no difference between reduced and detailed mechanisms predictions at higher temperatures. However, the difference between the reduced model and detailed model predictions was higher at lower temperatures.

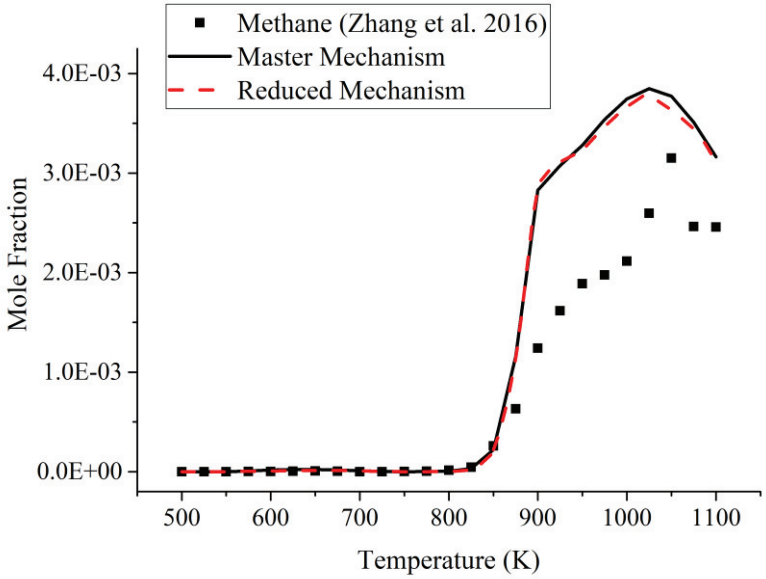

Figure 4.60. Validation of the skeletal mechanism on methane mole fraction with JSR

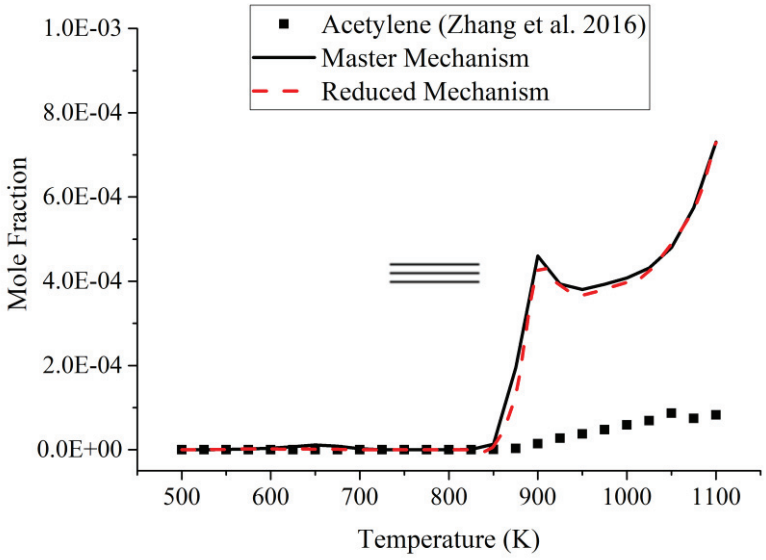

Figure 4.61. Validation of the skeletal mechanism on acetylene mole fraction with JSR

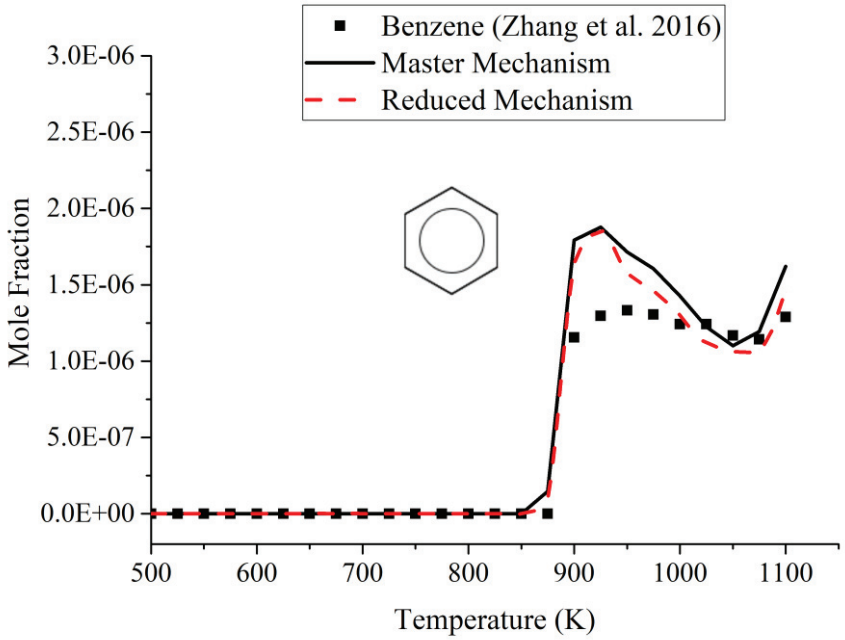

Figure 4.62. Validation of the skeletal mechanism on benzene mole fraction with JSR

As seen from Figure 4.63 to Figure 4.68 the skeletal mechanism mole fraction predictions of experimental conditions of flame of Bakali et al. (1998) were highly identical to the predictions of the master mechanism.

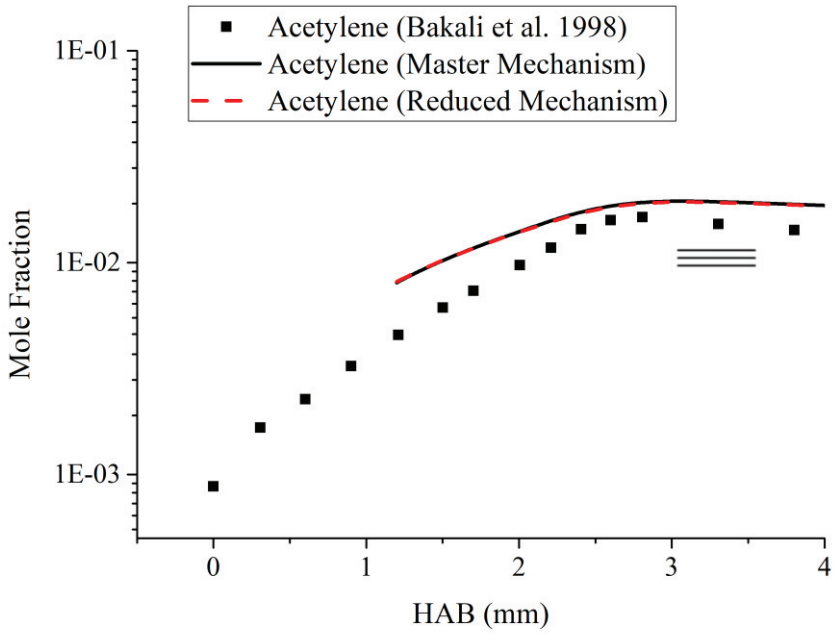

Figure 4.63. Validation of the skeletal mechanism with acetylene mole fraction profile of a flame

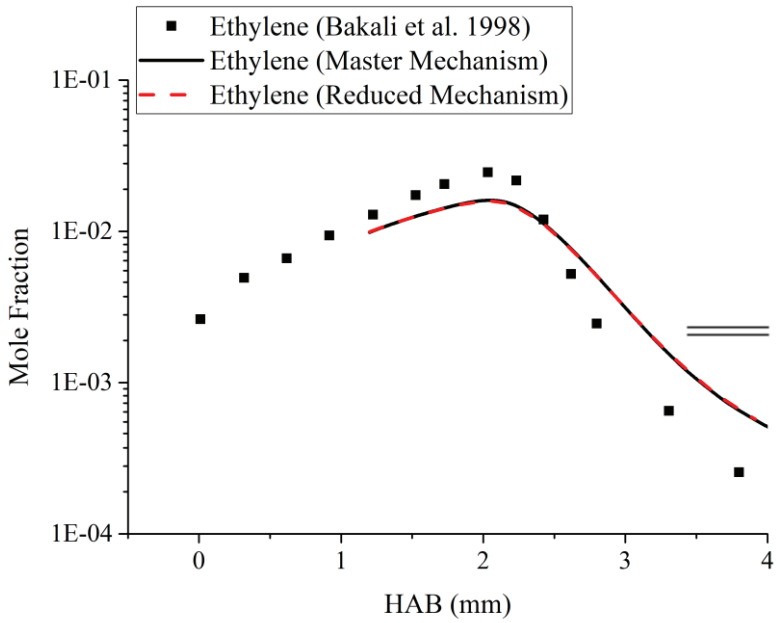

Figure 4.64. Validation of the skeletal mechanism with ethylene mole fraction profile of a flame

There was no noticeable difference for acetylene and ethylene mole fraction predictions of reduced and master mechanisms on the flame of Bakali et al. (1998). It can be deduced that, the most of the reactions that are significant to designate the premixed flame products were not eliminated at the mechanism reduction part.

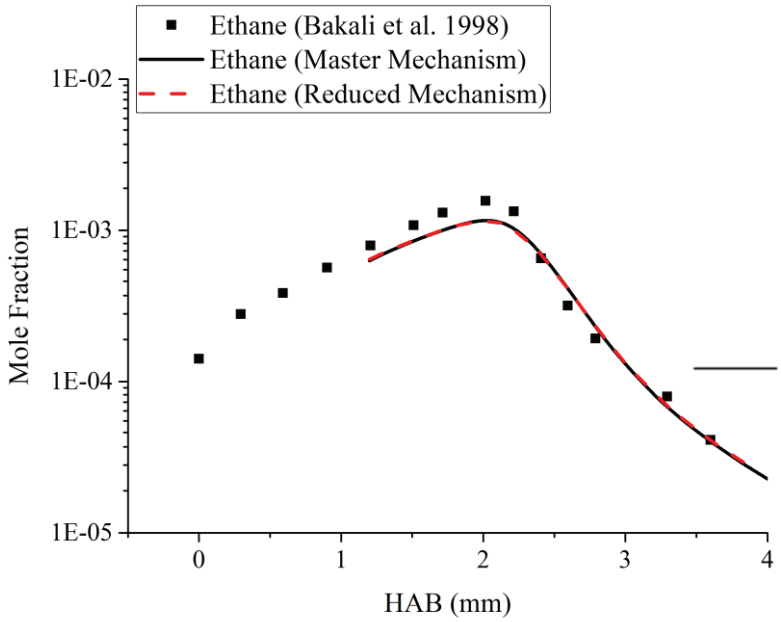

Figure 4.65. Validation of the skeletal mechanism with ethane mole fraction profile of a flame

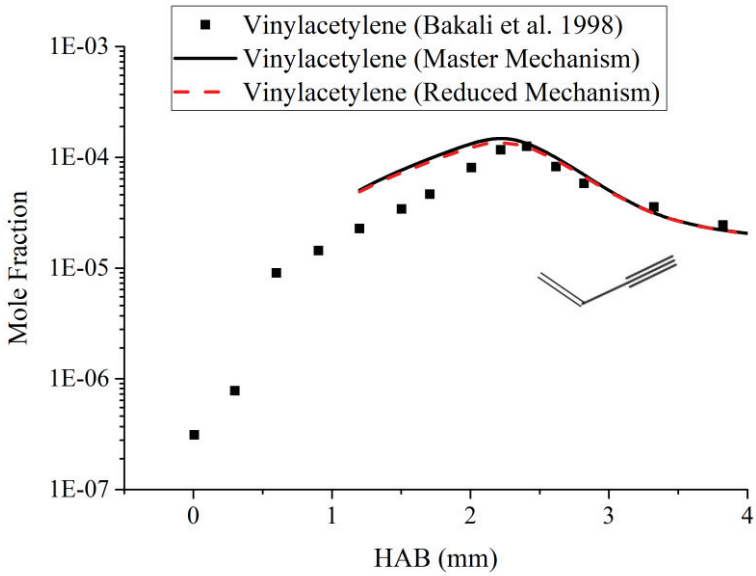

Figure 4.66. Validation of the skeletal mechanism with vinylacetylene mole fraction profile of a flame

The reduced mechanism predictions were almost same as the master mechanism predictions for ethane and vinylacetylene as seen from Figure 4.65. and Figure 4.66. respectively. There was a slight difference between reduced mechanism and master mechanism predictions especially at lower HAB for diacetylene. The reduced mechanism predictions and master mechanism predictions were almost identical for benzene flame (Figure 4.68.).

Validations of reduced mechanism in terms of ignition delay time were done for two shock-tube experimental data with stoichiometric fuel/air ratio (Figure 4.69). For 20 bar pressure, the reduced mechanism predictions of the ignition delay time were very close to the master mechanism predictions at temperatures higher than 1050 K. However, for lower temperatures (720K to 1050 K) the difference between reduced model and detailed model were slightly increased. The largest difference between reduced and detailed model was a factor of around 1.5 which correspond to the temperatures of 770K to 950 K for the shock tube operated at 20 bar pressure. For 38 bar pressure, the difference between the reduced model and the experimental data was highly greater than the difference between master mechanism predictions a and the experimental data. For higher temperatures (1050 K to 1176 K) the difference between the reduced model and the detailed model were smaller. The maximum difference for the reduced model predictions and shock-tube experimental data was around factor of 2.4 for 38 bar at ~950 K.

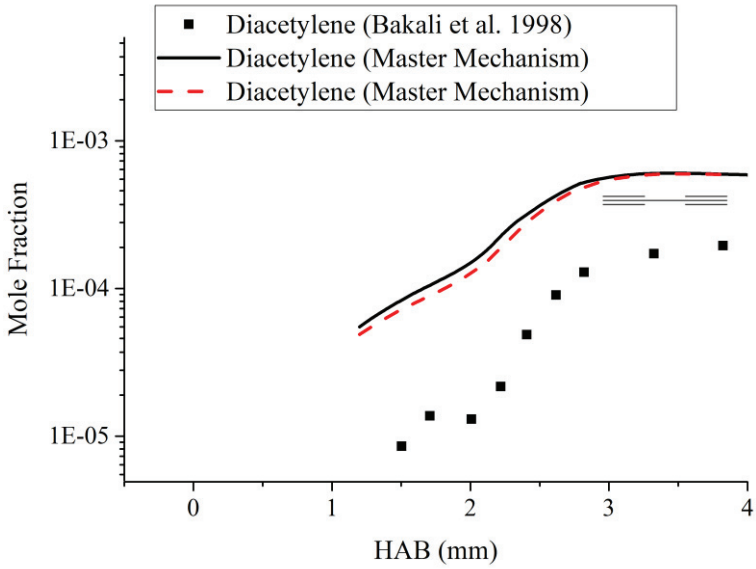

Figure 4.67. Validation of the skeletal mechanism with diacetylene mole fraction profile of a flame

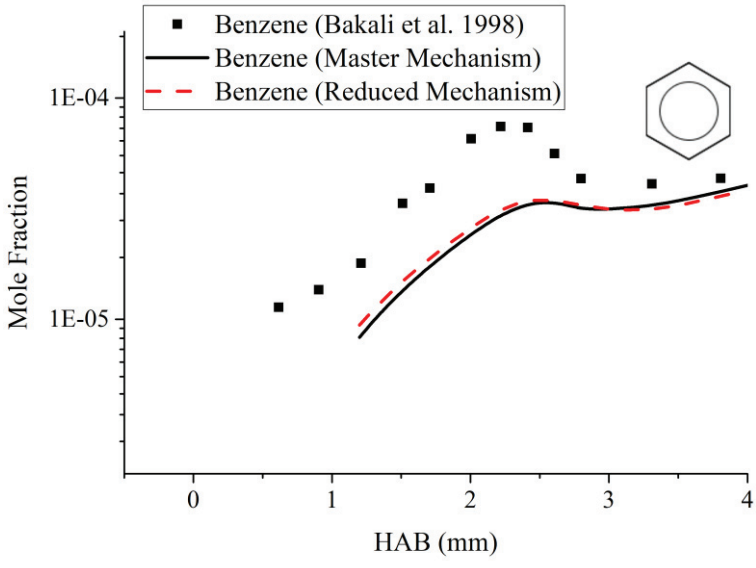

Figure 4.68. Validation of the skeletal mechanism with benzene mole fraction profile of a flame

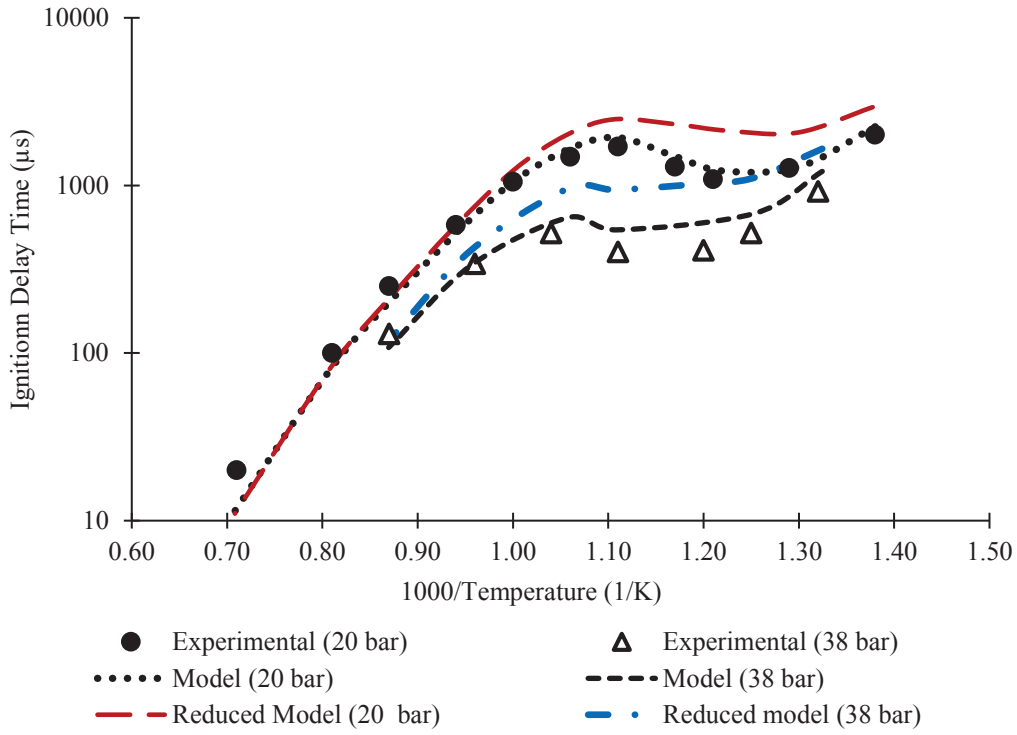

Figure 4.69. Validations of the reduced mechanism by ignition delay time

The validations of the skeletal mechanism were shown that, it is possible to use the skeletal mechanism instead of master mechanism when the computational power is limited. However, the ignition delay time predictions at low temperatures were found as more sensitive to the removed reactions.

4.5. Comparison of the Detailed and Skeletal Mechanism on Flame

In this section, the detailed and skeletal mechanism predictions of species mole fractions were compared with the experimental data from the flame of Inal and Senkan (2002).

As seen from Figure 4.70. and Figure 4.71, the predictions of detailed and skeletal mechanisms were similar for both n-heptane and hydrogen mole fractions. There was almost no difference between the predictions of the acetylene, propadiene and 1,3-butadiene mole fractions of detailed and skeletal mechanism as seen from Figure 4.72, Figure 4.73 and Figure 4.74 respectively. For benzene, the difference between detailed and skeletal mechanism predictions were greater than the previous species (Figure 4.75). However, the maximum difference between the detailed and reduced model was less than

a factor of around 1.2. For toluene, naphthalene, phenanthrene, and pyrene there were not a noticeable difference between the reduced and detailed model estimations as seen from Figure 4.76, Figure 4.77, Figure 4.78 and Figure 4.79, respectively.

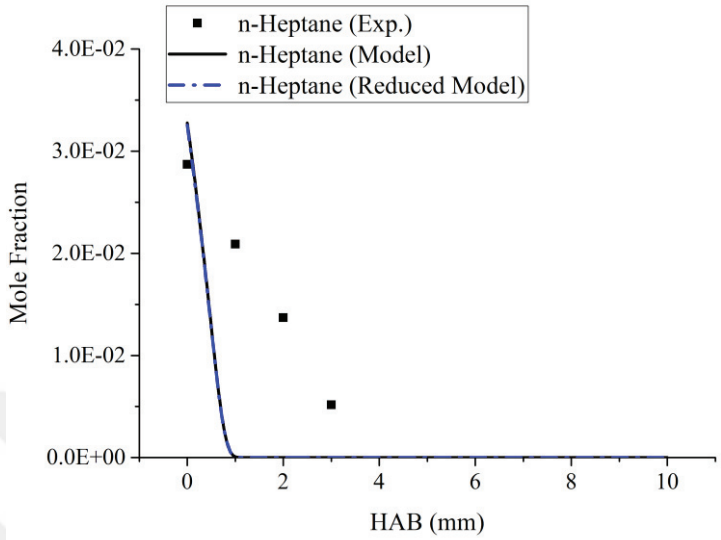

Figure 4.70. Comparison of detailed and skeletal mechanism n-heptane mole fraction predictions on the flame

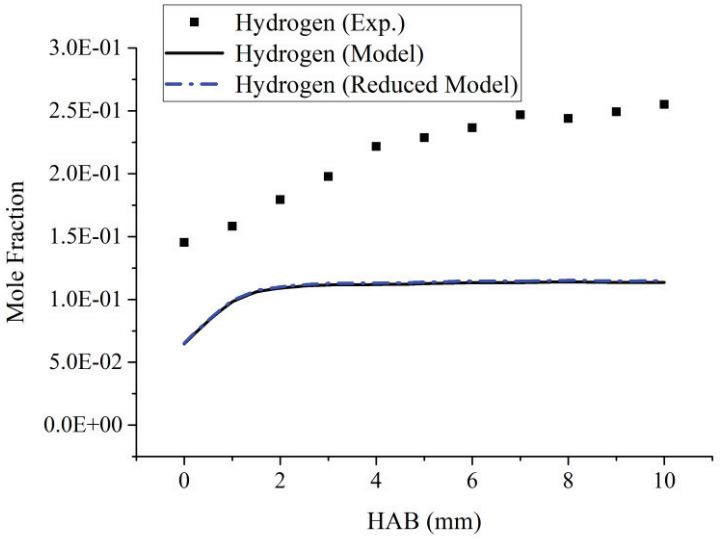

Figure 4.71. Comparison of detailed and skeletal mechanism hydrogen mole fraction predictions on the flame

As a result of the comparisons between reduced and detailed mechanism predictions at various conditions, it can be said that the skeletal mechanism was almost as capable as detailed mechanism for flame simulations. The reactions and their rate

parameters for the skeletal kinetic mechanism was given in Table B 2. in Appendices B in digital format.

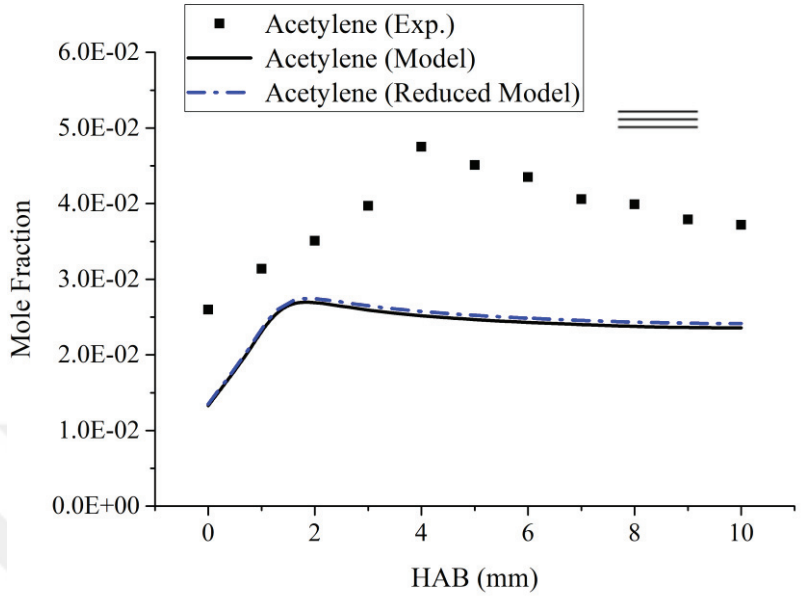

Figure 4.72. Comparison of detailed and skeletal mechanism acetylene mole fraction predictions on the flame

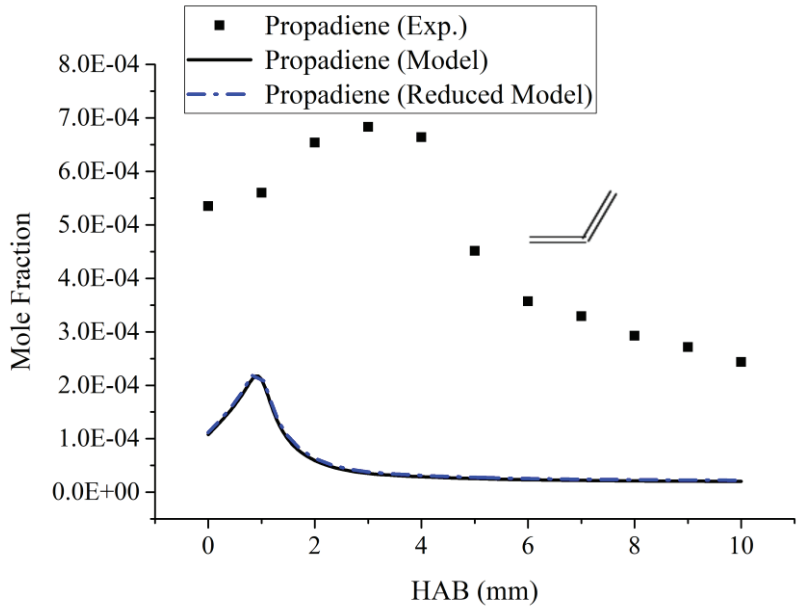

Figure 4.73. Comparison of detailed and skeletal mechanism propadiene mole fraction predictions on the flame

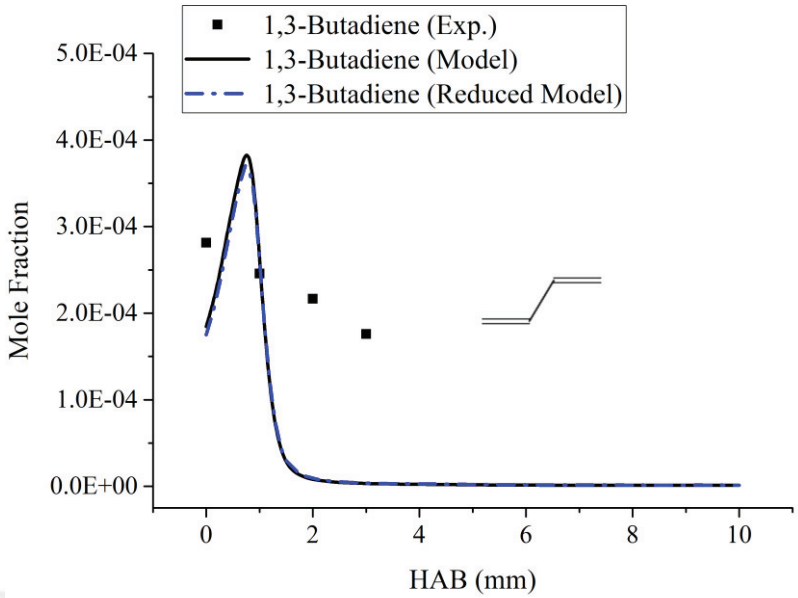

Figure 4.74. Comparison of detailed and skeletal mechanism 1,3-butadiene mole fraction predictions on the flame

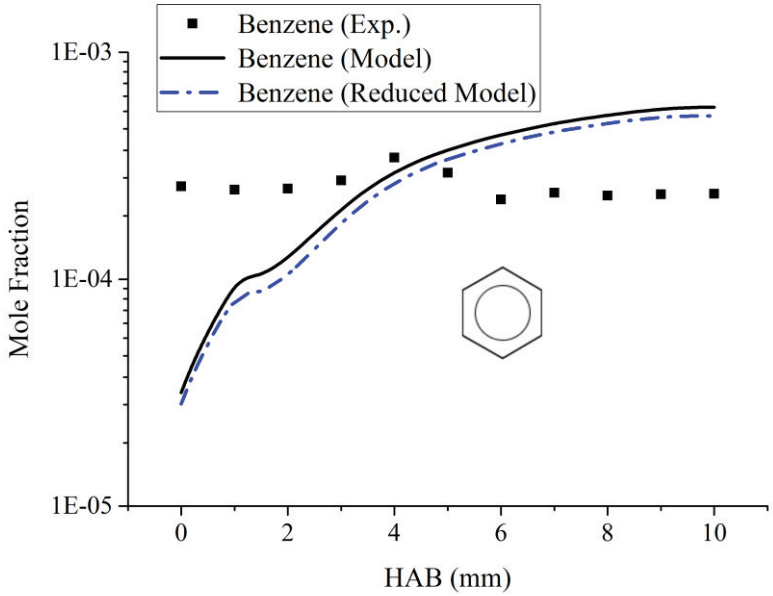

Figure 4.75. Comparison of detailed and skeletal mechanism benzene mole fraction predictions on the flame

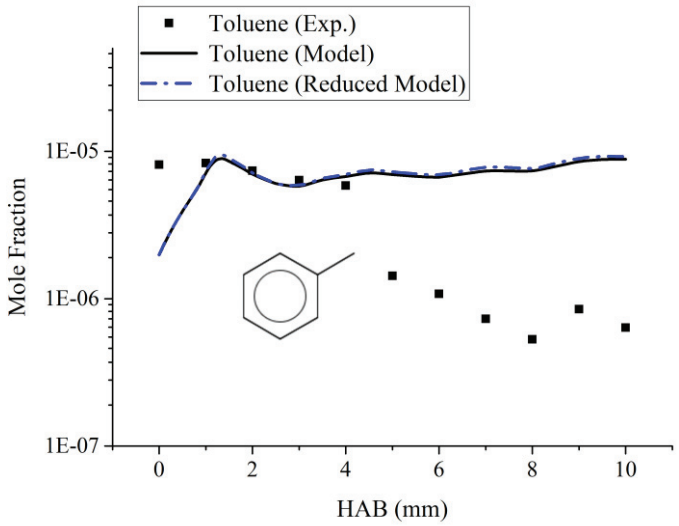

Figure 4.76. Comparison of detailed and skeletal mechanism toluene mole fraction predictions on the flame

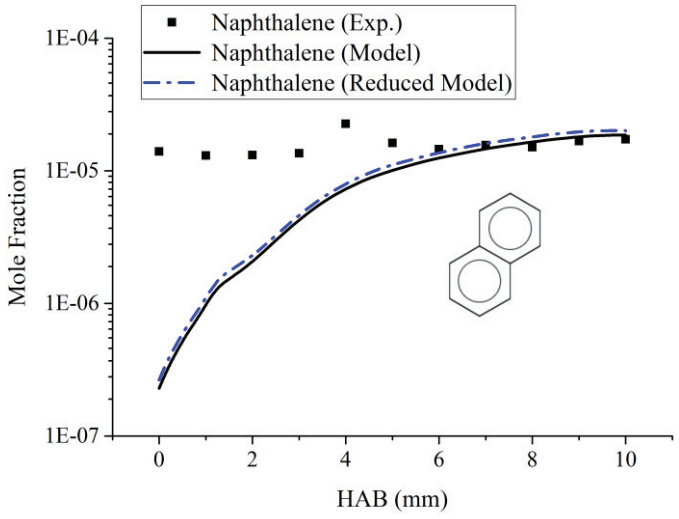

Figure 4.77. Comparison of detailed and skeletal mechanism naphthalene mole fraction predictions on the flame

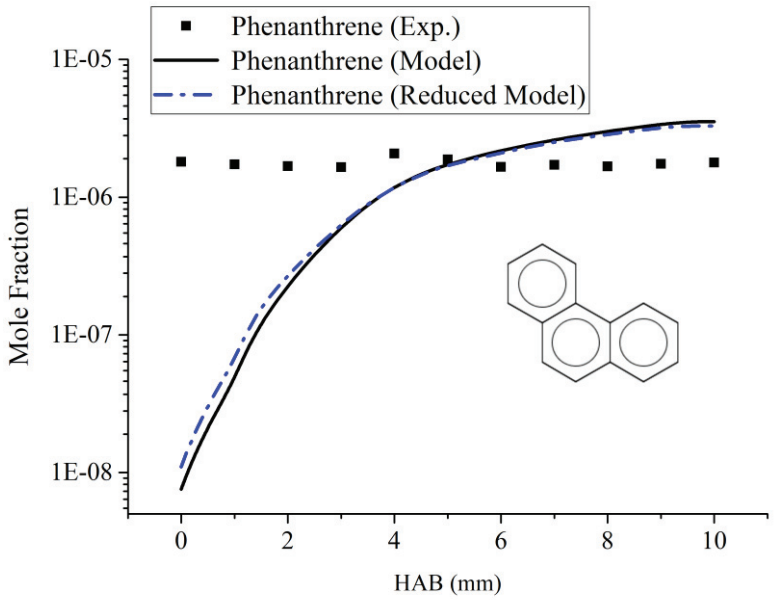

Figure 4.78. Comparison of detailed and skeletal mechanism phenanthrene mole fraction predictions on the flame

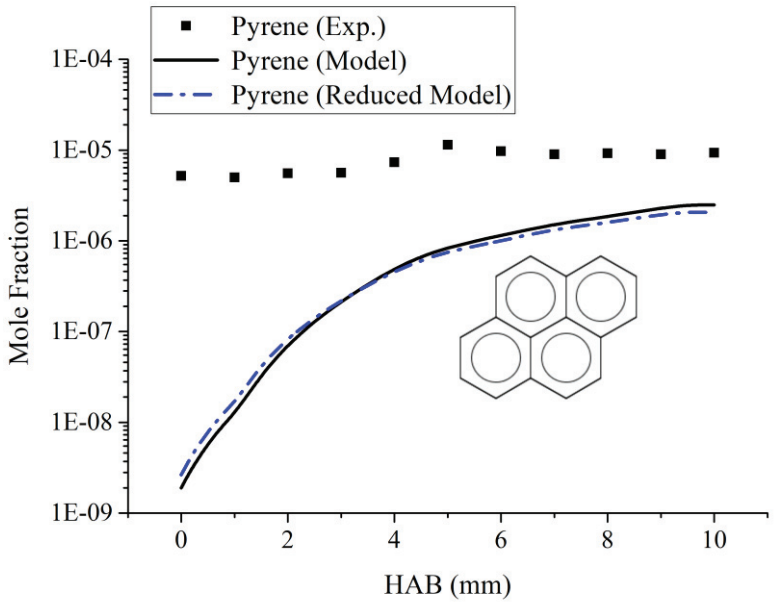

Figure 4.79. Comparison of detailed and skeletal mechanism pyrene mole fraction predictions on the flame

CHAPTER 5

CONCLUSION

To clarify the oxidation characteristics of n-heptane, burner stabilized premixed laminar fuel-rich n-heptane flame was modeled by using Detailed chemical kinetic modeling (DCKM). DCKM technique was used to study combustion kinetics of n-heptane at fuel-rich condition. A detailed chemical kinetic mechanism was generated by merging various mechanisms. The base mechanism was about the detailed decomposition pathways of n-heptane in wide range of conditions. Donor mechanisms covers the formation pathways of polycyclic aromatic hydrocarbons. Depending on sensitivity analysis, some reaction rate parameters were changed to achieve good agreement with the experimental data. The resulting detailed mechanism consists of 4185 reactions and 893 species. Generated mechanism was validated by experimental data of jet stirred reactor (JSR), premixed flame species mole fractions, ignition delay time measurements in shock-tube. The mechanism predicted most of the stable products of the fuel-rich premixed n-heptane flame. Detailed analyses of the n-heptane flame were done by rate of production, sensitivity and pathway analyses. As a result of sensitivity analysis, most sensitive reactions across the flame were found as $H+O_2=O+OH$ and $H_2+O=OH+H$ for most of the species, those reactions determine the amount of the free radicals on the flame. Formation of first aromatic ring and polycyclic hydrocarbons (PAHs) were also investigated on the n- heptane flame. By the rate of production and reaction pathway analyses it was seen that propargyl radical (C_3H_3), vinylacetylene (C_4H_4), and acetylene (C_2H_2) were the main precursors for the formation of benzene in n-heptane flame. For the formation of two membered aromatic ring, naphthalene, propargyl and acetylene were found to be main precursors. Phenanthrene which is a three membered PAH was mainly formed from cyclopentadienyl radical (C_5H_5), and phenyl radical under experimental conditions studies. For the formation of pyrene, indenyl radical and acetylene were found as the main precursors. A reduced mechanism was also generated to investigate the combustion behavior n-heptane with less computational effort. The skeletal mechanism was generated by directed relation graph with error propagation method, the skeletal mechanism consists of 1879 reactions and 359 species. The skeletal mechanism was in

good agreement with the detailed mechanism on the species mole fraction predictions of the n-heptane flame.

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APPENDIX A

SENSITIVITY ANALYSES FOR SELECTED SPECIES

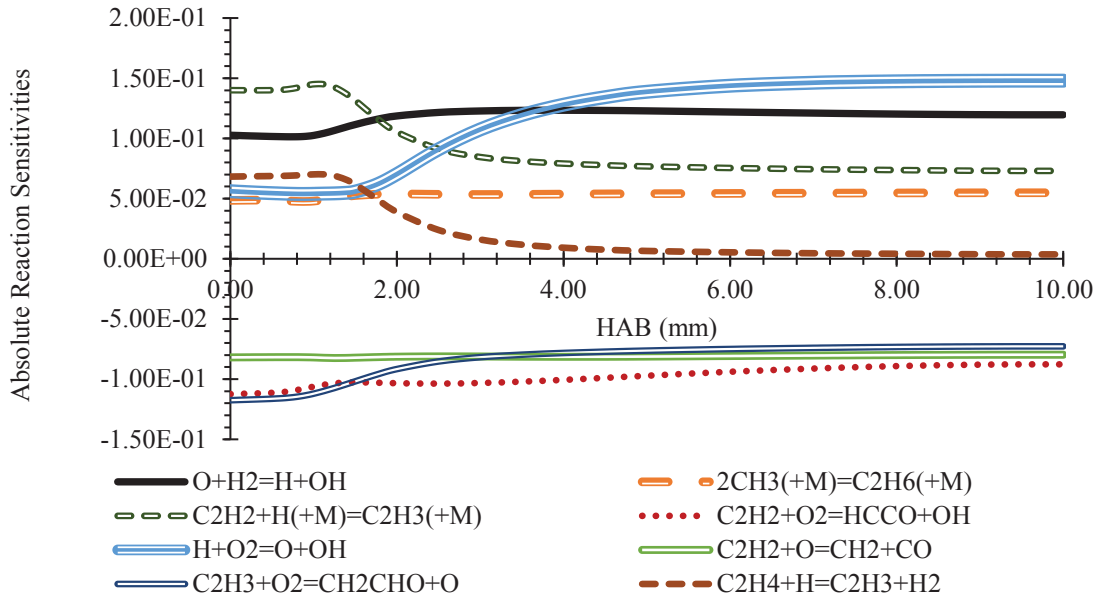

Figure A. 1. Sensitivity analysis of acetylene (C_2H_2) across the flame

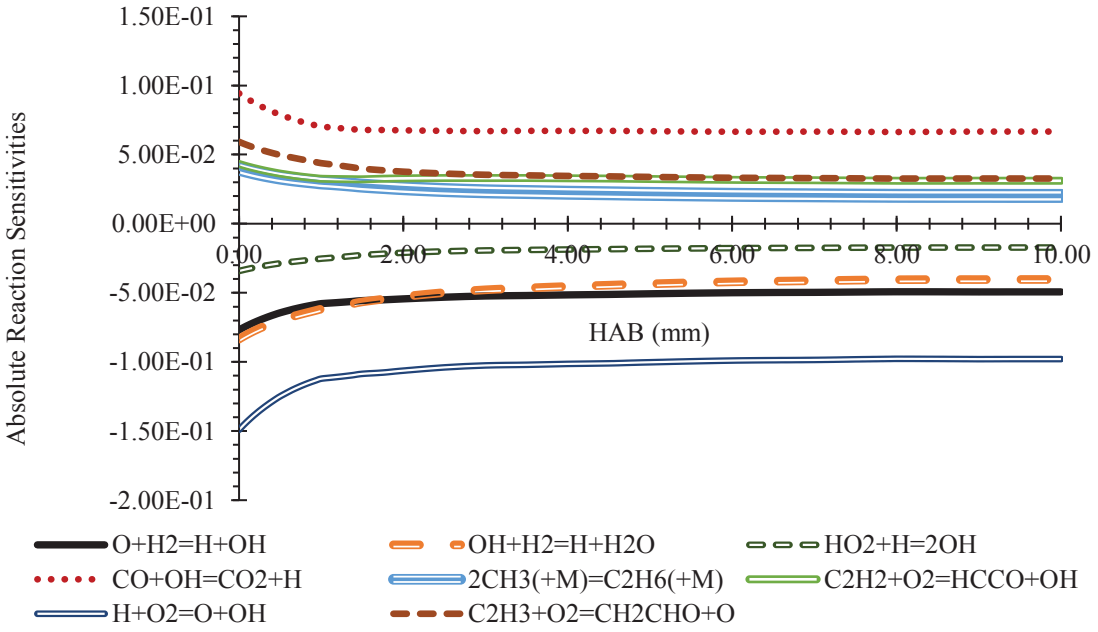

Figure A. 2. Sensitivity analysis of hydrogen (H_2) across the flame

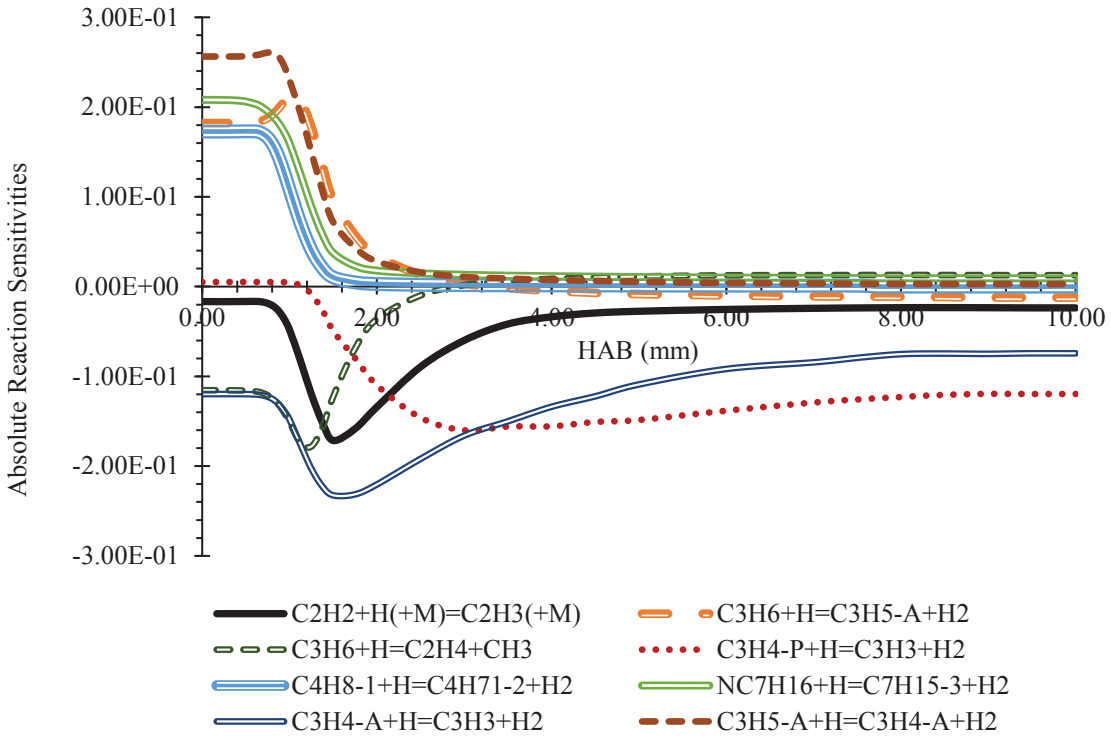

Figure A. 3. Sensitivity analysis of propadiene (C_3H_4-A) across the flame

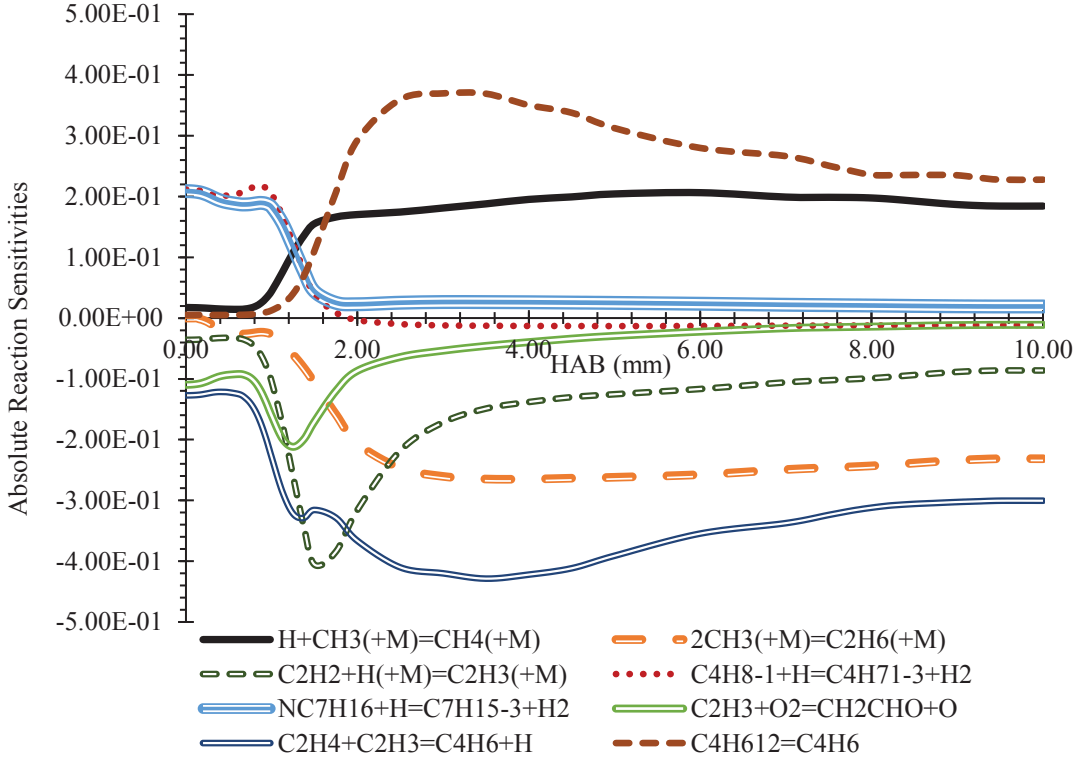

Figure A. 4. Sensitivity analysis of 1-3 butadiene across the flame

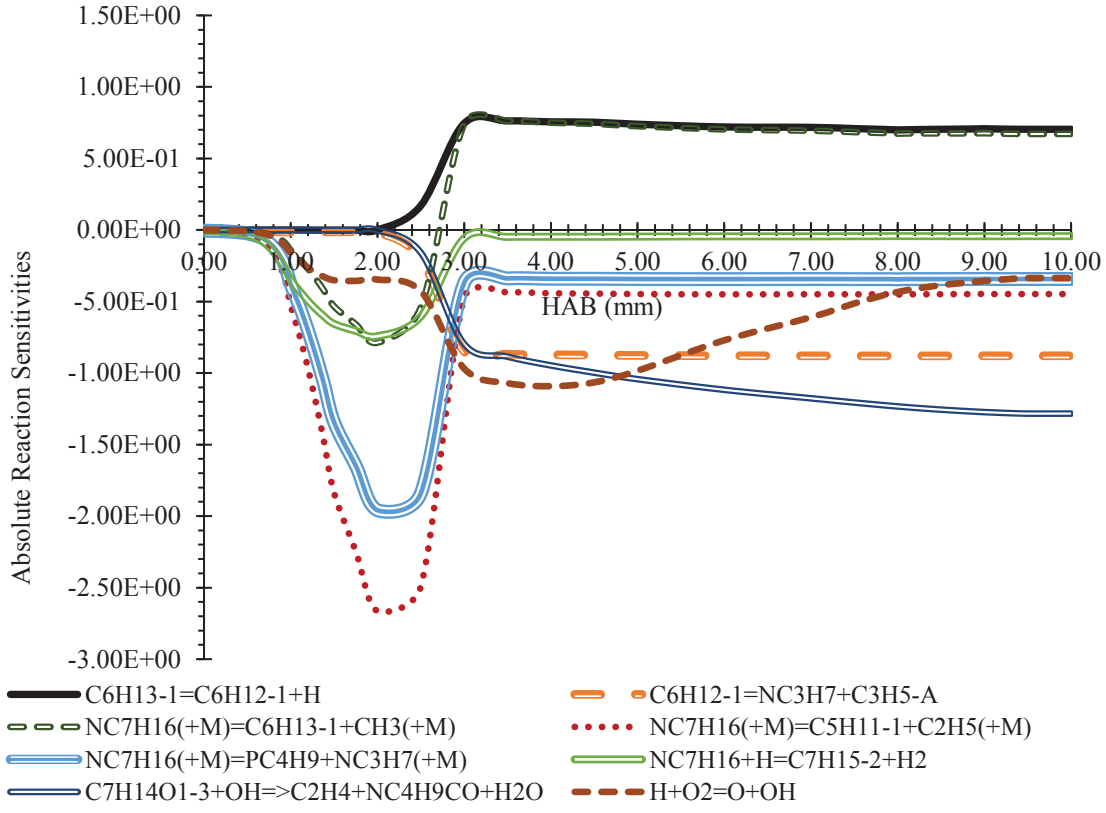

Figure A. 5. Sensitivity analysis of n-heptane across the flame

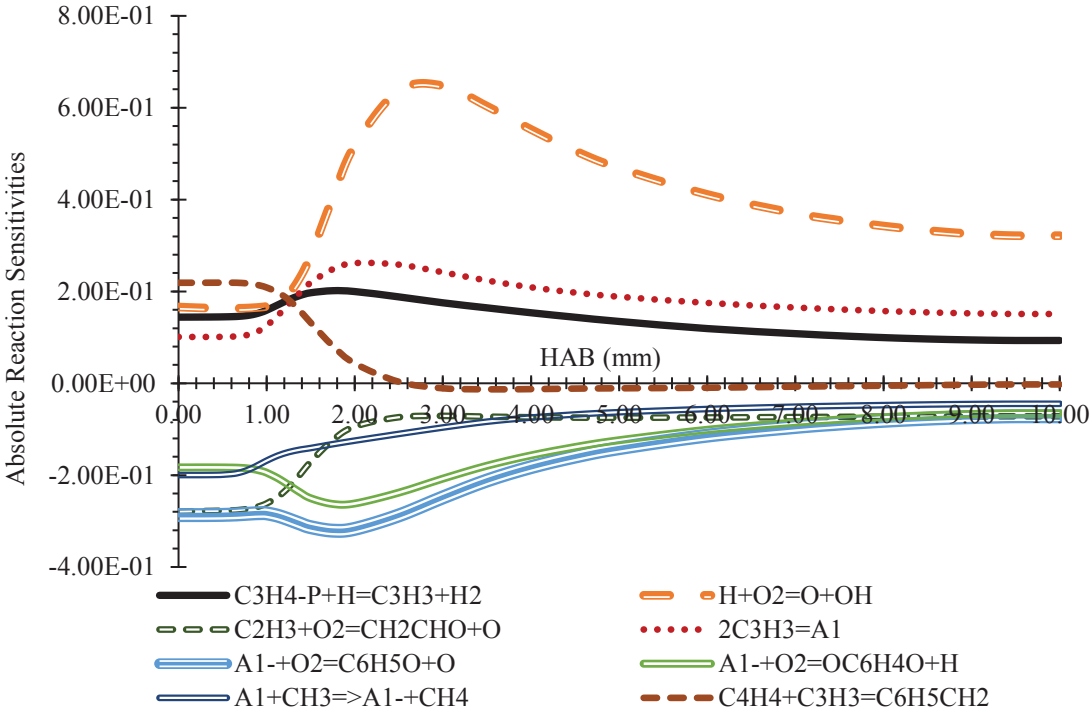

Figure A. 6. Sensitivity analysis of benzene across the flame

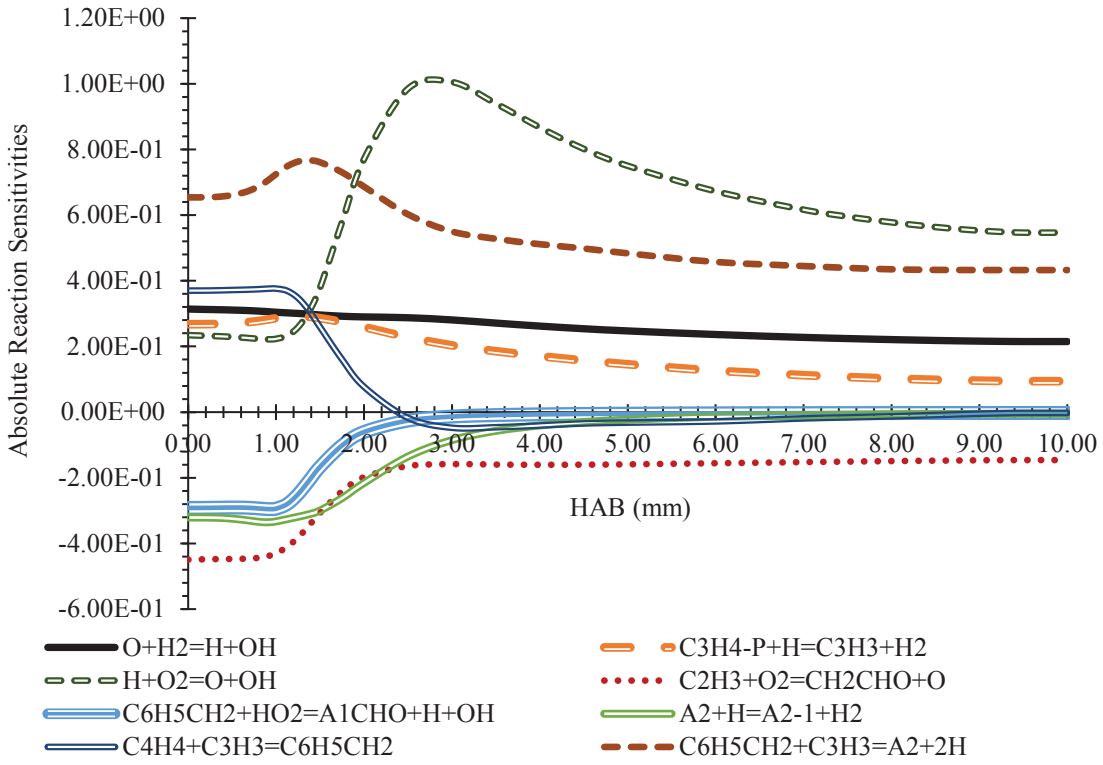

Figure A. 7. Sensitivity analysis of naphthalene across the flame

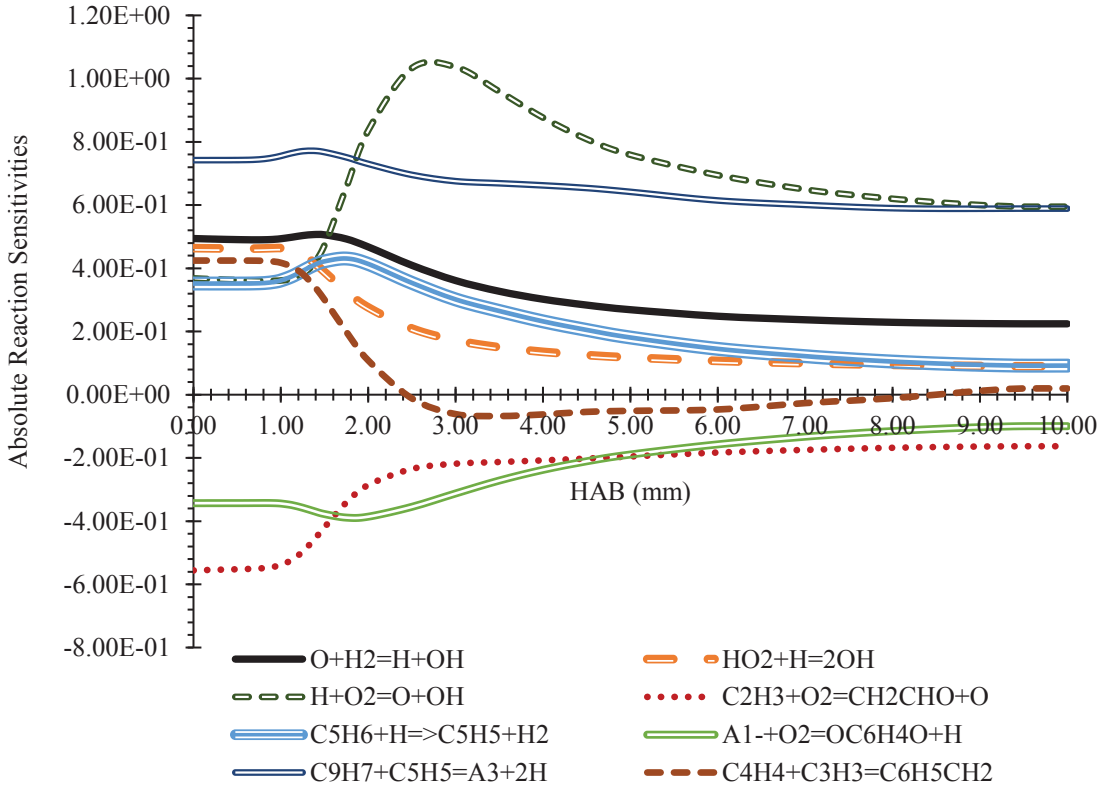

Figure A. 8. Sensitivity analysis of phenanthrene across the flame

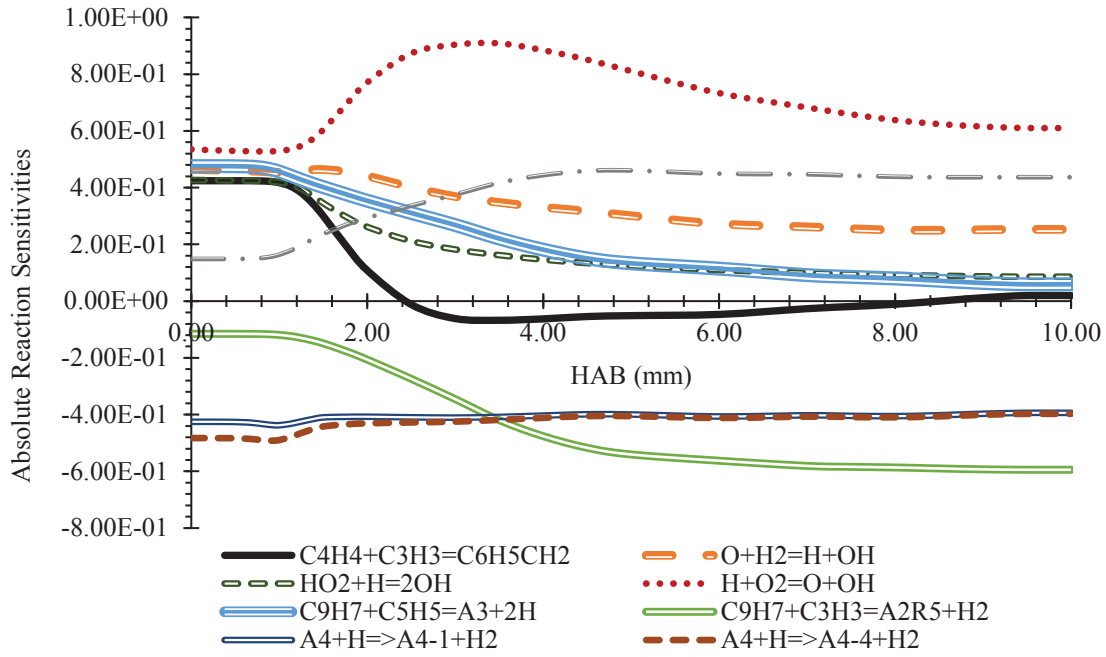

Figure A. 9. Sensitivity analysis of pyrene across the flame

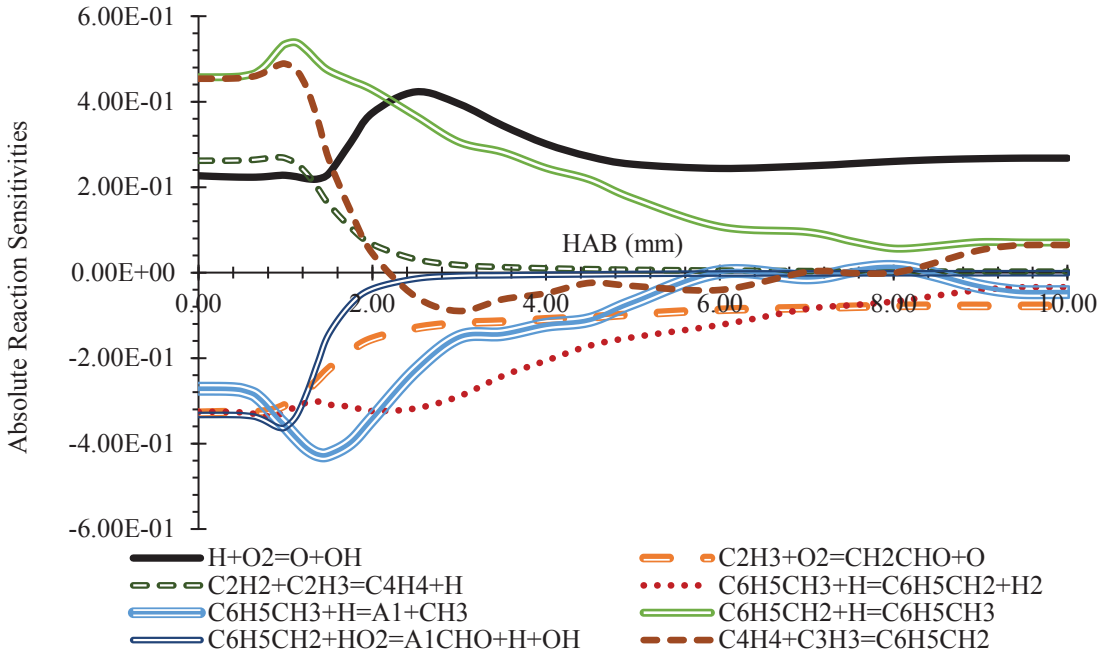

Figure A. 10. Sensitivity analysis of toluene across the flame

For most of the species H+O2=O+OH reaction was found as the most sensitive reaction on species mole fractions. In general, if the species were stable product, the H+O2=O+OH reaction was shown positive sensitivity which means right hand side of the reaction was more desirable for that stable species formation.

APPENDIX B

DETAILED AND SKELETAL KINETIC MECHANISM

Table B. 1. Detailed kinetic mechanism reactions and their rate parameters (pre-exponent factor, temperature exponent, and activation energy)

	Reactions	A (cm, s, mol units)	ß	Ea (cal/mol)	Additional Expressions
1	H+O2=O+OH	1.04E+14	0	15286	REV/2.637E4 2.651E0 4.88E3/
2	O+H2=H+OH	5.08E+04	2.67	6292	REV/2.29E9 1.404E0 1.832E4/
3	OH+H2=H+H2O	2.16E+08	1.51	3430	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.83/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.83/ REV/6.165E15 -5.0E-1 0.0E0/
4	O2+M=2O+M	4.42E+17	-0.634	118900	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.75/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.75/ REV/4.714E18 -1.0E0 0.0E0/
5	OH+M=O+H+M	9.78E+17	-0.743	102100	Third body: H2 /1.3/ Third body: H2O /14.0/ Third body: AR /0.67/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.67/ LOW/3.482E16 -4.11E-1 -1.115E3/ TROE/5.0E-1 1.0E-30 1.0E30 1.0E10/
6	H+O2(+M)=HO2(+M)	1.48E+12	0.6	0	REV/3.166E12 3.48E-1 5.551E4/
7	HO2+H=H2+O2	1.66E+13	0	823	REV/2.028E10 7.2E-1 3.684E4/
8	HO2+H=2OH	7.08E+13	0	295	REV/3.217E12 3.29E-1 5.328E4/
9	HO2+O=OH+O2	3.25E+13	0	0	REV/3.989E10 1.204E0 6.925E4/
10	HO2+OH=H2O+O2	1.97E+10	0.962	-328.4	REV/1.03E14 0.0E0 1.104E4/ DUP
11	H2O2+O2=2HO2	1.14E+16	-0.347	49730	REV/1.94E11 0.0E0 -1.409E3/ DUP
12	H2O2+O2=2HO2	2.14E+13	-0.347	37280	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.64/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.64/ LOW/1.202E17 0.0E0 4.55E4/ TROE/5.0E-1 1.0E-30 1.0E30 1.0E10/

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Table B .1. (cont.)

13	H2O2(+M)=2OH(+M)	2.95E+14	0	48430	REV/3.716E7 1.695E0 2.2E4/
14	H2O2+H=H2+HO2	2.15E+10	1	6000	REV/8.568E3 2.676E0 1.856E4/
15	H2O2+O=OH+HO2	9.55E+06	2	3970	Third body: H2 /2.0/ Third body: O2 /6.0/ Third body: H2O /6.0/ Third body: AR /0.5/ Third body: CO /1.5/ Third body: CO2 /3.5/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.5/ LOW/1.35E24 -2.788E0 4.191E3/
16	CO+O(+M)=CO2(+M)	1.80E+10	0	2384	
17	CO+OH=CO2+H	6.00E+10	0.2161	-260.5	REV/2.28E16 -4.7E-1 8.497E4/
18	CO+HO2=CO2+OH	3.01E+13	0	23000	Third body: H2 /2.0/ Third body: H2O /12.0/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ REV/3.582E10 1.041E0 -4.573E2/
19	HCO+M=H+CO+M	4.75E+11	0.66	14870	REV/1.198E12 3.09E-1 3.395E4/
20	HCO+O2=CO+HO2	7.58E+12	0	410	REV/2.212E12 6.56E-1 8.823E4/
21	HCO+H=CO+H2	7.34E+13	0	0	REV/4.725E11 6.38E-1 8.682E4/
22	HCO+O=CO+OH	3.02E+13	0	0	REV/1.241E18 -5.53E-1 1.122E5/
23	HCO+O=CO2+H	3.00E+13	0	0	REV/3.259E13 5.51E-1 1.031E5/
24	HCO+OH=CO+H2O	1.02E+14	0	0	REV/7.286E14 2.11E-1 8.977E4/
25	HCO+CH3=CH4+CO	2.65E+13	0	0	REV/8.07E15 0.0E0 5.342E4/
26	HCO+HO2=CH2O+O2	2.50E+14	-0.061	13920	
27	HCO+HO2=>CO2+H+OH	3.00E+13	0	0	REV/1.2E11 0.0E0 -1.1E3/
28	O2CHO=HCO+O2	9.96E+15	-1.126	41000	REV/3.908E14 -9.09E-1 1.181E4/
29	CH2O+O2CHO=HCO+HO2CHO	1.99E+12	0	11660	REV/3.856E8 1.532E0 -6.372E3/
30	HO2CHO=OCHO+OH	5.01E+14	0	40150	REV/7.5E13 0.0E0 2.9E4/
31	OCHO+M=H+CO2+M	5.32E+14	-0.353	17580	REV/1.8E13 0.0E0 0.0E0/
32	CH2O+CO=2HCO	9.19E+13	0.37	73040	
33	2HCO=>H2+2CO	3.00E+12	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.35E24 -2.57E0 1.425E3/ TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
34	HCO+H(+M)=CH2O(+M)	1.09E+12	0.48	-260	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/5.07E27 -3.42E0 8.4348E4/ TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
35	CO+H2(+M)=CH2O(+M)	4.30E+07	1.5	79600	REV/4.896E6 1.811E0 2.903E4/

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Table B .1. (cont.)

36	CH2O+OH=HCO+H2O	7.82E+07	1.63	-1055	REV/3.39E5 2.187E0 1.793E4/
37	CH2O+H=HCO+H2	5.74E+07	1.9	2740	REV/1.919E7 1.418E0 1.604E4/
38	CH2O+O=HCO+OH	6.26E+09	1.15	2260	REV/4.5E15 -1.1E0 0.0E0/
39	HOCH2O=CH2O+OH	2.06E+21	-2.336	25730	REV/1.123E15 -2.95E-1 1.15E4/
40	HOCH2O=HOCHO+H	1.00E+14	0	14900	REV/2.255E3 2.093E0 5.289E4/
41	HOCHO=CO+H2O	2.45E+12	0	60470	REV/6.772E5 1.008E0 5.147E4/
42	HOCHO=CO2+H2	2.95E+09	0	48520	REV/1.0E14 0.0E0 0.0E0/
43	HOCHO=HCO+OH	3.47E+22	-1.542	110700	REV/3.5E10 0.0E0 -3.275E3/
44	HOCHO+O2=OCHO+HO2	4.10E+12	-0.308	59880	
45	HOCHO+OH=>H2O+CO2+H	2.62E+06	2.06	916	
46	HOCHO+OH=>H2O+CO+OH	1.85E+07	1.51	-962	
47	HOCHO+H=>H2+CO2+H	4.24E+06	2.1	4868	
48	HOCHO+H=>H2+CO+OH	6.03E+13	-0.35	2988	
49	HOCHO+CH3=>CH4+CO+OH	3.90E-07	5.8	2200	REV/2.4E12 0.0E0 1.0E4/
50	HOCHO+HO2=OCHO+H2O2	2.55E+12	0.04	34470	
51	HOCHO+HO2=>H2O2+CO+OH	1.00E+12	0	11920	
52	HOCHO+O=>CO+2OH	1.77E+18	-1.9	2975	REV/5.6E12 0.0E0 1.36E4/
53	HOCHO+HCO=CH2O+OCHO	8.58E+11	0.04	26750	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ LOW/1.867E25 -3.0E0 2.4307E4/ TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
54	CH3O(+M)=CH2O+H(+M)	6.80E+13	0	26170	REV/8.393E10 7.4E-2 1.771E4/
55	CH2O+CH3O=CH3OH+HCO	6.62E+11	0	2294	REV/1.44E1 3.1E0 6.935E3/
56	CH4+CH3O=CH3+CH3OH	6.12E+02	2.867	8248	REV/6.749E13 2.18E-1 8.281E4/
57	CH3O+CH3=CH2O+CH4	1.20E+13	0	0	REV/1.074E12 -3.1E-2 6.527E4/
58	CH3O+HO2=CH2O+H2O2	3.01E+11	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ LOW/1.27E32 -4.82E0 6.53E3/ TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
59	CH2O+H(+M)=CH2OH(+M)	5.40E+11	0.454	3600	REV/1.975E14 -5.8E-1 2.006E4/ DUP
60	CH2OH+O2=CH2O+HO2	1.51E+15	-1	0	REV/3.152E13 4.2E-1 2.508E4/ DUP
61	CH2OH+O2=CH2O+HO2	2.41E+14	0	5017	REV/1.732E14 7.3E-2 5.875E4/
62	CH2OH+HO2=CH2O+H2O2	1.20E+13	0	0	REV/7.602E14 4.81E-1 5.956E4/
63	CH2OH+HCO=2CH2O	1.80E+14	0	0	REV/1.285E13 5.55E-1 7.498E4/
64	CH2OH+CH3O=CH2O+CH3OH	2.40E+13	0	0	REV/9.63E3 2.9E0 1.311E4/
65	CH2OH+CH2O=CH3OH+HCO	1.88E+04	2.722	4208	REV/3.0E12 0.0E0 0.0E0/
66	CH2O+CH3OH=2CH2OH	6.50E+12	0.659	68460	REV/8.169E13 -2.4E-2 3.347E4/
67	CH2OH+HO2=HOCH2O+OH	1.00E+13	0	0	REV/1.5E11 0.0E0 1.19E4/
68	OCH2O2H=CH2O+HO2	1.28E+18	-1.8	10460	REV/4.241E8 9.5E-1 2.62E4/

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Table B .1. (cont.)

69	OCH2O2H=HOCH2O2	3.00E+11	0	8600	REV/1.046E14 -8.4E-1 3.487E4/
70	HOCH2O2+HO2=HOCH2O2H+O2	3.50E+10	0	-3275	REV/1.0E13 0.0E0 0.0E0/
71	HOCH2O2H=HOCH2O+OH	1.02E+21	-1.92	42490	LOW/2.95E44 -7.35E0 9.546E4/ TROE/4.14E-1 2.79E2 5.459E3 1.0E10/
72	CH3OH(+M)=CH3+OH(+M)	1.90E+16	0	91730	LOW/2.34E40 -6.33E0 1.031E5/ TROE/7.73E-1 6.93E2 5.333E3 1.0E10/
73	CH3OH(+M)=CH2OH+H(+M)	2.69E+16	-0.08	98940	REV/1.386E4 2.509E0 8.871E3/
74	CH3OH+H=CH2OH+H2	1.20E+06	2.4	2583	REV/2.319E3 2.59E0 7.956E3/
75	CH3OH+O=CH2OH+OH	3.88E+05	2.5	3080	REV/1.758E5 2.003E0 2.034E4/
76	CH3OH+OH=CH2OH+H2O	1.44E+06	2	-839	REV/1.238E12 -2.39E-1 -3.501E3/
77	CH3OH+O2=CH2OH+HO2	2.05E+13	0	44900	REV/7.195E4 1.963E0 8.19E2/
78	CH3OH+HO2=CH2OH+H2O2	1.08E+04	2.55	10530	REV/3.351E2 2.833E0 1.5E4/
79	CH3OH+CH3=CH2OH+CH4	3.19E+01	3.17	7172	REV/7.416E10 -1.04E-1 1.059E4/
80	CH3O+CH3OH=CH2OH+CH3OH	3.00E+11	0	4074	REV/6.03E13 0.0E0 0.0E0/
81	CH3OH+CH2O=2CH3O	7.98E+12	0.452	81490	Third body: H2 /2.0/ Third body: CO /2.0/ Third body: CO2 /3.0/ Third body: H2O /5.0/ LOW/6.4E23 -1.8E0 0.0E0/ SRI/4.5E-1 7.97E2 9.79E2 1.0E0 0.0E0/
82	H+CH3(+M)=CH4(+M)	1.20E+15	-0.4	0	REV/6.73E2 2.946E0 8.047E3/
83	CH4+H=CH3+H2	6.14E+05	2.5	9587	REV/6.776E2 2.94E0 1.554E4/
84	CH4+OH=CH3+H2O	5.83E+04	2.6	2190	REV/5.804E5 1.927E0 5.648E3/
85	CH4+O=CH3+OH	1.02E+09	1.5	8600	REV/7.166E0 3.491E0 3.468E3/
86	CH4+HO2=CH3+H2O2	1.13E+01	3.74	21010	REV/1.736E6 1.868E0 1.298E4/
87	CH4+CH2=2CH3	2.46E+06	2	8270	REV/1.654E16 -8.55E-1 1.039E3/
88	CH3+OH=CH2(S)+H2O	4.51E+17	-1.34	1417	REV/1.5E12 5.0E-1 -1.1E2/
89	CH3+OH=CH3O+H	6.94E+07	1.343	11200	REV/1.65E11 6.5E-1 -2.84E2/
90	CH3+OH=CH2OH+H	3.09E+07	1.596	4506	REV/9.224E5 2.072E0 1.406E4/
91	CH3+OH=CH2+H2O	5.60E+07	1.6	5420	REV/6.19E12 1.47E-1 2.455E4/
92	CH3+HO2=CH3O+OH	1.00E+12	0.269	-687.5	REV/2.018E7 2.132E0 5.321E4/
93	CH3+HO2=CH4+O2	1.16E+05	2.23	-3022	REV/3.83E15 -1.47E-1 6.841E4/
94	CH3+O=CH2O+H	5.54E+13	0.05	-136	REV/4.718E14 -4.51E-1 2.88E2/
95	CH3+O2=CH3O+O	7.55E+12	0	28320	REV/5.285E-1 3.477E0 5.992E4/
96	CH3+O2=CH2O+OH	2.64E+00	3.283	8105	LOW/6.85E24 -3.0E0 0.0E0/ TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
97	CH3+O2(+M)=CH3O2(+M)	7.81E+09	0.9	0	REV/1.323E14 -8.53E-1 9.259E3/
98	CH3O2+CH2O=CH3O2H+HCO	1.99E+12	0	11660	REV/2.233E12 -6.94E-1 -6.55E2/
99	CH4+CH3O2=CH3+CH3O2H	1.81E+11	0	18480	REV/2.346E14 -1.031E0 2.404E3/
100	CH3OH+CH3O2=CH2OH+CH3O2H	1.81E+12	0	13710	REV/1.967E12 1.76E-1 2.807E4/
101	CH3O2+CH3=2CH3O	5.08E+12	0	-1411	REV/5.302E14 -7.92E-1 3.552E4/

(cont. on next page)

Table B .1. (cont.)

102	CH3O2+HO2=CH3O2H+O2	2.47E+11	0	-1570	
103	2CH3O2=>CH2O+CH3OH+O2	3.11E+14	-1.61	-1051	
104	2CH3O2=>O2+2CH3O	1.40E+16	-1.61	1860	REV/1.72E9 1.019E0 4.078E4/
105	CH3O2+H=CH3O+OH	9.60E+13	0	0	REV/2.229E11 6.28E-1 5.752E4/
106	CH3O2+O=CH3O+O2	3.60E+13	0	0	REV/1.536E13 4.34E-1 5.916E4/
107	CH3O2+OH=CH3OH+O2	6.00E+13	0	0	REV/2.514E6 1.883E0 -2.875E3/
108	CH3O2H=CH3O+OH	6.31E+14	0	42300	REV/4.488E12 -1.3E-2 9.02E3/
109	CH2(S)=CH2	1.00E+13	0	0	REV/5.067E12 -1.45E-1 1.316E4/
110	CH2(S)+CH4=2CH3	1.60E+13	0	-570	
111	CH2(S)+O2=>CO+OH+H	7.00E+13	0	0	REV/2.022E16 -5.91E-1 1.527E4/
112	CH2(S)+H2=CH3+H	7.00E+13	0	0	REV/6.948E13 -2.53E-1 1.248E4/
113	CH2(S)+H=CH+H2	3.00E+13	0	0	
114	CH2(S)+O=>CO+2H	3.00E+13	0	0	REV/1.154E18 -7.7E-1 8.523E4/
115	CH2(S)+OH=CH2O+H	3.00E+13	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/3.2E27 -3.14E0 1.23E3/ TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
116	CH2+H(+M)=CH3(+M)	2.50E+16	-0.8	0	REV/5.955E14 -3.65E-1 6.098E4/
117	CH2+O2=CH2O+O	2.40E+12	0	1500	
118	CH2+O2=>CO+OH+H	5.00E+12	0	1500	
119	CH2+O=>CO+2H	5.00E+13	0	0	REV/5.16E18 -1.8E0 3.46E3/ DUP
120	CH2+H=CH+H2	1.00E+18	-1.56	0	REV/6.183E8 1.655E0 2.135E4/
121	CH2+OH=CH+H2O	1.13E+07	2	3000	REV/9.371E12 1.61E-1 7.121E4/
122	CH+O2=HCO+O	3.30E+13	0	0	REV/1.356E15 0.0E0 1.543E5/
123	C+OH=CO+H	5.00E+13	0	0	REV/1.07E14 0.0E0 1.382E5/
124	C+O2=CO+O	5.00E+13	0	0	REV/2.774E15 0.0E0 1.76E5/
125	CH+O=CO+H	5.70E+13	0	0	REV/5.069E14 0.0E0 8.811E4/
126	CH+OH=HCO+H	3.00E+13	0	0	REV/1.897E11 6.7E-1 2.873E4/ DUP
127	CH2+H=CH+H2	2.70E+11	0.67	25700	REV/8.372E14 0.0E0 5.752E4/
128	CH+H2O=H+CH2O	1.71E+13	0	-755	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.135E36 -5.246E0 1.705E3/ TROE/4.05E-1 1.12E3 6.96E1 1.0E10/

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Table B .1. (cont.)

129	2CH3(+M)=C2H6(+M)	9.21E+16	-1.17	635.8	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.99E41 -7.08E0 6.685E3/ TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
130	C2H5+H(+M)=C2H6(+M)	5.21E+17	-0.99	1580	REV/1.062E4 2.582E0 9.76E3/
131	C2H6+H=C2H5+H2	1.15E+08	1.9	7530	REV/1.702E2 3.063E0 6.648E3/
132	C2H6+O=C2H5+OH	3.55E+06	2.4	5830	REV/1.45E4 2.476E0 1.807E4/
133	C2H6+OH=C2H5+H2O	1.48E+07	1.9	950	REV/2.921E10 3.34E-1 -5.93E2/
134	C2H6+O2=C2H5+HO2	6.03E+13	0	51870	REV/1.273E-8 6.236E0 9.817E3/
135	C2H6+CH3=C2H5+CH4	1.51E-07	6	6047	REV/1.849E0 3.597E0 3.151E3/
136	C2H6+HO2=C2H5+H2O2	3.46E+01	3.61	16920	REV/2.017E1 3.182E0 1.734E3/
137	C2H6+CH3O2=C2H5+CH3O2H	1.94E+01	3.64	17100	REV/4.779E8 4.69E-1 9.547E3/
138	C2H6+CH3O=C2H5+CH3OH	2.41E+11	0	7090	REV/1.969E9 9.21E-1 -1.49E3/
139	C2H6+CH=C2H5+CH2	1.10E+14	0	-260	REV/3.203E12 9.1E-2 1.75E4/
140	CH2(S)+C2H6=CH3+C2H5	1.20E+14	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.2E42 -7.62E0 6.97E3/ TROE/9.75E-1 2.1E2 9.84E2 4.374E3/
141	C2H4+H(+M)=C2H5(+M)	1.08E+12	0.454	1822	REV/1.688E18 -1.14E0 8.434E3/
142	H2+CH3O2=H+CH3O2H	1.50E+14	0	26030	REV/1.691E18 -1.14E0 8.438E3/
143	H2+C2H5O2=H+C2H5O2H	1.50E+14	0	26030	REV/4.82E14 0.0E0 7.153E4/
144	C2H5+C2H3=2C2H4	6.86E+11	0.11	-4300	REV/2.39E6 2.4E0 6.669E4/
145	CH3+C2H5=CH4+C2H4	1.18E+04	2.45	-2921	REV/2.029E9 1.028E0 1.051E4/
146	C2H5+H=2CH3	9.69E+13	0	220	REV/1.033E17 -5.0E-1 7.742E4/
147	C2H5+O=CH3CHO+H	1.10E+14	0	0	REV/9.68E15 -7.23E-1 2.765E4/
148	C2H5+HO2=C2H5O+OH	1.10E+13	0	0	REV/4.404E14 -4.25E-1 3.089E4/
149	CH3O2+C2H5=CH3O+C2H5O	8.00E+12	0	-1000	REV/1.322E8 6.15E-1 3.413E4/
150	C2H5O+O2=CH3CHO+HO2	4.28E+10	0	1097	REV/3.0E11 0.0E0 6.336E3/
151	C2H5O=CH3+CH2O	1.32E+20	-2.018	20750	REV/8.0E12 0.0E0 6.4E3/
152	C2H5O=CH3CHO+H	5.43E+15	-0.687	22230	REV/2.876E56 -1.382E1 1.462E4/
153	C2H5O2=C2H5+O2	1.31E+62	-14.784	49180	REV/1.325E14 -8.53E-1 9.263E3/
154	C2H5O2+CH2O=C2H5O2H+HCO	1.99E+12	0	11660	REV/2.237E12 -6.94E-1 -6.51E2/
155	CH4+C2H5O2=CH3+C2H5O2H	1.81E+11	0	18480	REV/2.35E14 -1.031E0 2.408E3/
156	CH3OH+C2H5O2=CH2OH+C2H5O2H	1.81E+12	0	13710	REV/3.763E13 -7.92E-1 3.382E4/

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Table B .1. (cont.)

157	C2H5O2+HO2=C2H5O2H+O2	1.75E+10	0	-3275	REV/8.957E0 3.302E0 1.838E3/
158	C2H6+C2H5O2=C2H5+C2H5O2H	8.60E+00	3.76	17200	REV/5.661E8 1.033E0 -1.705E3/
159	C2H5O2H=C2H5O+OH	6.31E+14	0	42300	REV/1.814E45 -1.15E1 1.46E4/
160	C2H4O2H=C2H5+O2	4.37E+47	-12.115	31020	REV/3.633E13 -6.26E-1 3.984E4/
161	C2H5+O2=C2H4O1-2+OH	1.63E+11	-0.31	6150	REV/2.247E3 2.301E0 6.597E4/
162	C2H5+O2=CH3CHO+OH	8.27E+02	2.41	5285	REV/1.203E36 -8.13E0 2.702E4/
163	C2H5O2=C2H4O2H	2.28E+39	-8.479	45170	REV/1.502E36 -9.345E0 6.984E4/
164	C2H5O2=CH3CHO+OH	2.52E+41	-10.2	43710	REV/4.632E32 -7.438E0 1.67E4/
165	C2H5O2=C2H4+HO2	1.82E+38	-8.45	37890	REV/1.959E40 -9.812E0 4.471E4/
166	C2H5O2=C2H4O1-2+OH	4.00E+43	-10.46	45580	REV/8.199E30 -5.781E0 3.793E4/
167	C2H4O2H=C2H4O1-2+OH	8.85E+30	-6.08	20660	REV/1.922E32 -6.587E0 2.021E4/
168	C2H4O2H=C2H4+HO2	3.98E+34	-7.25	23250	REV/1.339E32 -8.514E0 7.348E4/
169	C2H4O2H=CH3CHO+OH	1.19E+34	-9.02	29210	REV/1.006E4 1.549E0 -2.75E3/
170	C2H4O1-2=CH3+HCO	3.63E+13	0	57200	REV/9.013E10 2.07E-1 8.08E4/
171	C2H4O1-2=CH3CHO	7.41E+12	0	53800	REV/1.347E10 6.93E-1 2.474E4/
172	C2H4O1-2+OH=C2H3O1-2+H2O	1.78E+13	0	3610	REV/5.71E9 7.99E-1 1.592E4/
173	C2H4O1-2+H=C2H3O1-2+H2	8.00E+13	0	9680	REV/4.666E11 1.04E-1 2.067E4/
174	C2H4O1-2+HO2=C2H3O1-2+H2O2	1.13E+13	0	30430	REV/9.078E12 -3.41E-1 1.907E4/
175	C2H4O1-2+CH3O2=C2H3O1-2+CH3O2H	1.13E+13	0	30430	REV/9.093E12 -3.41E-1 1.908E4/
176	C2H4O1-2+C2H5O2=C2H3O1-2+C2H5O2H	1.13E+13	0	30430	REV/6.967E10 3.53E-1 1.961E4/
177	C2H4O1-2+CH3=C2H3O1-2+CH4	1.07E+12	0	11830	REV/1.839E8 5.86E-1 1.322E4/
178	C2H4O1-2+CH3O=C2H3O1-2+CH3OH	1.20E+11	0	6750	REV/1.002E14 4.1E-2 4.871E4/
179	C2H3O1-2=CH3CO	8.50E+14	0	14000	REV/1.245E15 -3.75E-1 4.401E4/
180	C2H3O1-2=CH2CHO	1.00E+14	0	14000	REV/1.75E13 0.0E0 0.0E0/
181	CH3CHO=CH3+HCO	7.69E+20	-1.342	86950	REV/1.639E10 6.33E-1 1.76E4/
182	CH3CHO+H=CH3CO+H2	2.37E+13	0	3642	REV/2.133E9 6.14E-1 1.441E4/
183	CH3CHO+O=CH3CO+OH	5.94E+12	0	1868	REV/2.472E10 5.27E-1 2.823E4/
184	CH3CHO+OH=CH3CO+H2O	3.37E+12	0	-619	REV/1.092E11 2.85E-1 -1.588E3/
185	CH3CHO+O2=CH3CO+HO2	3.01E+13	0	39150	REV/4.468E-4 4.767E0 1.746E4/
186	CH3CHO+CH3=CH3CO+CH4	7.08E-04	4.58	1966	REV/1.205E12 -6.2E-2 9.877E3/
187	CH3CHO+HO2=CH3CO+H2O2	3.01E+12	0	11920	REV/2.344E13 -5.07E-1 8.282E3/
188	CH3O2+CH3CHO=CH3O2H+CH3CO	3.01E+12	0	11920	REV/1.922E12 -1.0E-2 1.265E4/
189	CH3CHO+CH3CO3=CH3CO+CH3CO3H	3.01E+12	0	11920	REV/2.371E16 -1.277E0 2.375E4/
190	CH3CHO+OH=CH3+HOCHO	3.00E+15	-1.076	0	REV/1.332E5 2.511E0 2.495E4/
191	CH3CHO+OH=CH2CHO+H2O	1.72E+05	2.4	815	LOW/1.2E15 0.0E0 1.2518E4/
192	CH3CO(+M)=CH3+CO(+M)	3.00E+12	0	16720	REV/1.037E13 2.01E-1 6.056E4/

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Table B .1. (cont.)

193	CH3CO+H=CH2CO+H2	2.00E+13	0	0	REV/5.381E12 1.82E-1 5.914E4/
194	CH3CO+O=CH2CO+OH	2.00E+13	0	0	REV/2.364E16 -2.45E-1 6.21E4/
195	CH3CO+CH3=CH2CO+CH4	5.00E+13	0	0	REV/1.2E11 0.0E0 -1.1E3/
196	CH3CO3=CH3CO+O2	6.86E+19	-1.949	38530	REV/3.08E12 -2.94E-1 3.818E4/
197	CH3CO3+HO2=CH3CO3H+O2	1.75E+10	0	-3275	REV/3.845E12 5.3E-2 1.271E4/
198	H2O2+CH3CO3=HO2+CH3CO3H	2.41E+12	0	9936	REV/1.831E11 -1.96E-1 3.711E3/
199	CH4+CH3CO3=CH3+CH3CO3H	1.81E+11	0	18480	REV/1.085E13 -3.56E-1 1.362E4/
200	CH2O+CH3CO3=HCO+CH3CO3H	1.99E+12	0	11660	REV/1.45E12 4.0E-2 9.46E3/
201	C2H6+CH3CO3=C2H5+CH3CO3H	1.70E+13	0	20460	REV/3.618E7 1.761E0 1.338E3/
202	CH3CO3H=CH3CO2+OH	5.01E+14	0	40150	REV/4.548E8 1.378E0 1.752E4/
203	CH3CO2+M=CH3+CO2+M	4.40E+15	0	10500	
204	CH2CHO+O2=>CH2O+CO+OH	8.95E+13	-0.6	10120	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/2.69E33 -5.11E0 7.095E3/ TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
205	CH2+CO(+M)=CH2CO(+M)	8.10E+11	0	0	REV/1.434E11 4.7E-1 4.52E3/
206	CH2CO+H=HCCO+H2	2.00E+14	0	8000	REV/2.854E9 8.09E-1 4.944E4/
207	CH2CO+O=CH2+CO2	1.75E+12	0	1350	REV/3.723E9 4.52E-1 3.108E3/
208	CH2CO+O=HCCO+OH	1.00E+13	0	8000	REV/7.604E10 3.65E-1 1.341E4/
209	CH2CO+OH=HCCO+H2O	1.00E+13	0	2000	REV/3.75E14 2.17E-1 1.034E5/
210	CH2(S)+CH2CO=C2H4+CO	1.60E+14	0	0	
211	HCCO+OH=>H2+2CO	1.00E+14	0	0	
212	HCCO+O=>H+2CO	8.00E+13	0	0	REV/1.623E15 0.0E0 6.906E4/
213	CH+CH2O=H+CH2CO	9.46E+13	0	-515	REV/1.721E17 0.0E0 1.646E5/
214	CH+HCCO=CO+C2H2	5.00E+13	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.58E51 -9.3E0 9.78E4/ TROE/7.35E-1 1.8E2 1.035E3 5.417E3/
215	C2H4(+M)=C2H2+H2(+M)	8.00E+12	0.44	88770	REV/1.541E9 1.201E0 1.878E4/
216	C2H4+O=CH2CHO+H	4.99E+06	1.88	183	REV/1.908E0 3.76E0 3.28E3/
217	C2H4+CH3=C2H3+CH4	6.62E+00	3.7	9500	REV/8.138E8 2.93E-1 -7.83E2/
218	C2H4+CH3O=C2H3+CH3OH	1.20E+11	0	6750	REV/7.929E12 -6.34E-1 -8.167E3/
219	C2H4+CH3O2=C2H3+CH3O2H	2.23E+12	0	17190	REV/7.943E12 -6.34E-1 -8.163E3/
220	C2H4+C2H5O2=C2H3+C2H5O2H	2.23E+12	0	17190	REV/3.295E12 -1.36E-1 9.44E3/
221	C2H4+CH3CO3=C2H3+CH3CO3H	1.13E+13	0	30430	REV/3.385E13 -6.5E-2 4.166E4/

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Table B .1. (cont.)

222	C2H4+CH3O2=C2H4O1-2+CH3O	2.82E+12	0	17110	REV/7.638E15 -9.16E-1 4.283E4/
223	C2H4+C2H5O2=C2H4O1-2+C2H5O	2.82E+12	0	17110	REV/4.28E14 -3.64E-1 3.75E4/
224	C2H4+HO2=C2H4O1-2+OH	2.23E+12	0	17190	REV/3.573E14 0.0E0 5.548E4/
225	CH+CH4=C2H4+H	6.00E+13	0	0	REV/6.128E19 -1.223E0 7.305E4/
226	CH2(S)+CH3=C2H4+H	2.00E+13	0	0	Third body: H2 /2.0/ LOW/6.346E31 -4.664E0 3.78E3/ TROE/7.88E-1 -1.02E4 1.0E-30/
227	C2H2+H(+M)=C2H3(+M)	1.71E+10	1.266	2709	REV/3.994E27 -4.883E0 9.345E4/
228	C2H3+O2=CH2O+HCO	8.50E+28	-5.312	6500	REV/9.427E13 2.53E-1 6.924E4/
229	C2H3+H=C2H2+H2	9.64E+13	0	0	REV/5.184E13 1.47E-1 8.413E4/
230	C2H3+OH=C2H2+H2O	5.00E+12	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/3.75E33 -4.8E0 1.9E3/ TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
231	C2H+H(+M)=C2H2(+M)	1.00E+17	0	0	REV/2.039E6 1.541E0 3.227E4/
232	C2H2+O2=HCCO+OH	2.00E+08	1.5	30100	REV/3.023E15 -6.04E-1 -1.782E3/
233	O+C2H2=C2H+OH	4.60E+19	-1.4	28950	
234	C2H2+O=HCCO+H	9.03E+12	0	4532	
235	C2H2+OH=C2H+H2O	9.00E+13	0	12950	
236	C2H2+OH=CH2CO+H	2.18E-04	4.5	-1000	REV/3.495E-6 4.638E0 5.212E4/
237	C2H2+OH=CH3+CO	4.83E-04	4	-2000	REV/3.852E9 1.436E0 4.382E3/
238	OH+C2H2=H+HCCOH	5.04E+05	2.3	13500	REV/9.299E13 -2.9E-1 3.111E4/
239	H+HCCOH=H+CH2CO	1.00E+13	0	0	Third body: H2 /2.0/ Third body: H2O /5.0/ Third body: CO /2.0/ Third body: CO2 /3.0/ LOW/3.11E85 -1.884E1 1.131E5/ TROE/5.0E-1 5.5E2 8.25E2 6.1E3/
240	C2H5OH(+M)=CH2OH+CH3(+M)	2.00E+23	-1.68	96400	Third body: H2 /2.0/ Third body: H2O /5.0/ Third body: CO /2.0/ Third body: CO2 /3.0/ LOW/5.11E85 -1.88E1 1.1877E5/ TROE/5.0E-1 6.5E2 8.0E2 1.0E15/
241	C2H5OH(+M)=C2H5+OH(+M)	2.40E+23	-1.62	99540	Third body: H2O /5.0/ LOW/3.09E55 -1.092E1 6.2644E4/ TROE/8.97E-1 1.0E10 1.0E0 5.0E9/
242	C2H5OH(+M)=C2H4+H2O(+M)	1.32E+05	2.52	60660	Third body: H2O /5.0/ LOW/4.46E87 -1.942E1 1.1558E5/ TROE/9.0E-1 9.0E2 1.1E3 3.5E3/
243	C2H5OH(+M)=CH3CHO+H2(+M)	7.24E+11	0.095	91010	REV/2.192E10 2.78E-1 4.43E2/
244	C2H5OH+O2=PC2H4OH+HO2	2.00E+13	0	52800	REV/1.946E11 8.9E-2 4.879E3/
245	C2H5OH+O2=SC2H4OH+HO2	1.50E+13	0	50150	REV/4.012E8 9.2E-1 1.794E4/

(cont. on next page)

Table B .1. (cont.)

246	C2H5OH+OH=PC2H4OH+H2O	1.81E+11	0.4	717	REV/1.458E9 8.31E-1 2.393E4/
247	C2H5OH+OH=SC2H4OH+H2O	5.56E+10	0.5	-380	REV/7.32E9 9.06E-1 1.721E4/
248	C2H5OH+OH=C2H5O+H2O	1.50E+10	0.8	2534	REV/3.93E-1 3.826E0 9.484E3/
249	C2H5OH+H=PC2H4OH+H2	1.88E+03	3.2	7150	REV/4.429E2 2.967E0 1.284E4/
250	C2H5OH+H=SC2H4OH+H2	1.79E+05	2.53	3420	REV/2.467E3 2.742E0 4.188E3/
251	C2H5OH+H=C2H5O+H2	5.36E+04	2.53	4405	REV/2.877E3 2.481E0 2.827E3/
252	C2H5OH+HO2=PC2H4OH+H2O2	2.38E+04	2.55	16490	REV/8.589E12 -2.58E-1 9.419E3/
253	C2H5OH+HO2=SC2H4OH+H2O2	6.00E+12	0	16000	REV/6.658E13 -4.83E-1 7.782E3/
254	C2H5OH+HO2=C2H5O+H2O2	2.50E+12	0	24000	REV/2.894E4 2.036E0 4.88E2/
255	C2H5OH+CH3O2=PC2H4OH+CH3O2H	1.23E+04	2.55	15750	REV/2.284E5 1.847E0 2.574E3/
256	C2H5OH+CH3O2=SC2H4OH+CH3O2H	8.20E+03	2.55	10750	REV/1.295E15 -9.27E-1 6.187E3/
257	C2H5OH+CH3O2=C2H5O+CH3O2H	2.50E+12	0	24000	REV/1.052E-1 3.837E0 5.58E3/
258	C2H5OH+O=PC2H4OH+OH	9.69E+02	3.23	4658	REV/1.862E2 2.888E0 8.884E3/
259	C2H5OH+O=SC2H4OH+OH	1.45E+05	2.47	876	REV/3.488E-5 4.924E0 9.8E1/
260	C2H5OH+O=C2H5O+OH	1.46E-03	4.73	1727	REV/6.294E1 3.48E0 1.616E4/
261	C2H5OH+CH3=PC2H4OH+CH4	3.30E+02	3.3	12290	REV/4.498E1 3.361E0 1.859E4/
262	C2H5OH+CH3=SC2H4OH+CH4	1.99E+01	3.37	7634	REV/8.545E1 3.336E0 9.044E3/
263	C2H5OH+CH3=C2H5O+CH4	2.04E+00	3.57	7721	REV/6.995E10 0.0E0 2.699E4/
264	C2H5OH+C2H5=PC2H4OH+C2H6	5.00E+10	0	13400	REV/6.995E10 0.0E0 2.399E0/
265	C2H5OH+C2H5=SC2H4OH+C2H6	5.00E+10	0	10400	REV/4.17E20 -2.84E0 1.24E3/
266	PC2H4OH=C2H4+OH	1.05E+25	-3.99	30390	REV/2.742E12 4.62E-1 -4.7E2/
267	SC2H4OH+M=CH3CHO+H+M	1.00E+14	0	25000	REV/1.2E11 0.0E0 -1.1E3/
268	O2C2H4OH=PC2H4OH+O2	3.90E+16	-1	30000	
269	O2C2H4OH=>OH+2CH2O	3.13E+09	0	18900	REV/2.19E5 2.39E0 2.504E4/
270	SC2H4OH+O2=CH3CHO+HO2	3.81E+06	2	1641	LOW/7.013E89 -2.038E1 1.0715E5/ TROE/8.63E-1 1.0E10 4.164E2 3.29E9/
271	CH3COCH3(+M)=CH3CO+CH3(+M)	7.11E+21	-1.57	84680	REV/8.62E4 2.322E0 2.471E4/
272	CH3COCH3+OH=CH3COCH2+H2O	1.25E+05	2.483	445	REV/6.374E4 2.375E0 1.453E4/
273	CH3COCH3+H=CH3COCH2+H2	9.80E+05	2.43	5160	REV/1.732E10 1.37E-1 1.285E4/
274	CH3COCH3+O=CH3COCH2+OH	5.13E+11	0.211	4890	REV/2.35E13 -5.01E-1 2.069E4/
275	CH3COCH3+CH3=CH3COCH2+CH4	3.96E+11	0	9784	REV/6.06E11 -2.68E-1 1.606E4/
276	CH3COCH3+CH3O=CH3COCH2+CH3OH	4.34E+11	0	6460	REV/2.057E13 -4.03E-1 3.181E3/
277	CH3COCH3+O2=CH3COCH2+HO2	6.03E+13	0	48500	REV/6.397E14 -7.5E-1 1.383E4/
278	CH3COCH3+HO2=CH3COCH2+H2O2	1.70E+13	0	20460	REV/1.245E16 -1.195E0 1.223E4/
279	CH3COCH3+CH3O2=CH3COCH2+CH3O2H	1.70E+13	0	20460	REV/1.0E11 0.0E0 6.0E3/
280	CH3COCH2=CH2CO+CH3	1.00E+14	0	31000	REV/1.2E11 0.0E0 -1.1E3/
281	CH3COCH2O2=CH3COCH2+O2	2.02E+15	-0.956	24460	REV/1.995E10 0.0E0 1.0E4/

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Table B .1. (cont.)

282	CH3COCH3+CH3COCH2O2=CH3COCH2+CH3COCH2O2H	1.00E+11	0	5000	REV/2.512E10 0.0E0 1.01E4/
283	CH2O+CH3COCH2O2=HCO+CH3COCH2O2H	1.29E+11	0	9000	
284	HO2+CH3COCH2O2=>CH3COCH2O2H+O2	1.00E+12	0	0	REV/4.242E8 1.74E0 - 4.342E3/
285	CH3COCH2O2H=CH3COCH2O+OH	1.00E+16	0	43000	REV/1.0E11 0.0E0 1.19E4/
286	CH3COCH2O=CH3CO+CH2O	3.73E+20	-2.176	17260	REV/1.81E13 0.0E0 0.0E0/
287	C2H3CHO=C2H3+HCO	2.00E+24	-2.135	103400	REV/3.311E10 6.13E-1 2.268E4/
288	C2H3CHO+H=C2H3CO+H2	1.34E+13	0	3300	REV/7.618E9 5.94E-1 1.984E4/
289	C2H3CHO+O=C2H3CO+OH	5.94E+12	0	1868	REV/2.42E5 2.007E0 3.331E4/
290	C2H3CHO+OH=C2H3CO+H2O	9.24E+06	1.5	-962	REV/1.302E11 2.65E-1 5.391E3/
291	C2H3CHO+O2=C2H3CO+HO2	1.01E+13	0	40700	REV/4.303E12 -8.2E-2 1.53E4/
292	C2H3CHO+HO2=C2H3CO+H2O2	3.01E+12	0	11920	REV/5.878E6 1.947E0 2.683E4/
293	C2H3CHO+CH3=C2H3CO+CH4	2.61E+06	1.78	5911	REV/1.0E13 0.0E0 2.8E4/
294	C2H3CHO+C2H3=C2H3CO+C2H4	1.74E+12	0	8440	REV/5.304E10 4.01E-1 2.291E4/
295	C2H3CHO+CH3O=C2H3CO+CH3OH	1.00E+12	0	3300	REV/8.371E13 -5.27E-1 1.371E4/
296	C2H3CHO+CH3O2=C2H3CO+CH3O2H	3.01E+12	0	11920	REV/1.51E11 0.0E0 4.81E3/
297	C2H3CO=C2H3+CO	1.37E+21	-2.179	39410	REV/1.81E13 0.0E0 0.0E0/
298	C2H5CHO=C2H5+HCO	1.50E+27	-3.205	87040	REV/2.377E10 6.54E-1 1.813E4/
299	C2H5CHO+H=C2H5CO+H2	4.00E+13	0	4200	REV/1.542E9 6.36E-1 1.431E4/
300	C2H5CHO+O=C2H5CO+OH	5.00E+12	0	1790	REV/1.695E8 1.308E0 2.848E4/
301	C2H5CHO+OH=C2H5CO+H2O	2.69E+10	0.76	-340	REV/1.414E6 1.988E0 2.138E4/
302	C2H5CHO+CH3=C2H5CO+CH4	2.61E+06	1.78	5911	REV/9.626E11 -4.1E-2 1.153E4/
303	C2H5CHO+HO2=C2H5CO+H2O2	2.80E+12	0	13600	REV/1.276E10 4.42E-1 1.746E4/
304	C2H5CHO+CH3O=C2H5CO+CH3OH	1.00E+12	0	3300	REV/2.013E13 -4.85E-1 8.26E3/
305	C2H5CHO+CH3O2=C2H5CO+CH3O2H	3.01E+12	0	11920	REV/6.432E12 -2.8E-2 1.97E4/
306	C2H5CHO+C2H5=C2H5CO+C2H6	1.00E+12	0	8000	REV/3.02E11 0.0E0 1.816E4/
307	C2H5CHO+C2H5O=C2H5CO+C2H5OH	6.03E+11	0	3300	REV/2.017E13 -4.86E-1 8.264E3/
308	C2H5CHO+C2H5O2=C2H5CO+C2H5O2H	3.01E+12	0	11920	REV/3.131E10 3.06E-1 - 5.8E1/
309	C2H5CHO+O2=C2H5CO+HO2	1.01E+13	0	40700	REV/1.651E12 1.2E-2 1.263E4/
310	C2H5CHO+CH3CO3=C2H5CO+CH3CO3H	3.01E+12	0	11920	REV/3.198E12 1.48E-1 3.013E4/
311	C2H5CHO+C2H3=C2H5CO+C2H4	1.70E+12	0	8440	REV/1.51E11 0.0E0 4.81E3/
312	C2H5CO=C2H5+CO	2.46E+23	-3.208	17550	LOW/3.5E60 -1.156E1 1.01E5/ TROE/1.83E-1 1.3E0 1.3E4 6.71E9/
313	CH3OCH3(+M)=CH3+CH3O(+M)	7.25E+21	-0.94	80250	REV/7.853E4 2.236E0 2.121E4/
314	CH3OCH3+OH=CH3OCH2+H2O	6.32E+06	2	-651.7	REV/9.042E3 2.432E0 1.036E4/
315	CH3OCH3+H=CH3OCH2+H2	7.72E+06	2.09	3384	REV/4.712E5 1.683E0 7.81E3/
316	CH3OCH3+O=CH3OCH2+OH	7.75E+08	1.36	2250	REV/1.138E13 -3.53E-1 8.657E3/
317	CH3OCH3+HO2=CH3OCH2+H2O2	1.68E+13	0	17690	REV/2.215E14 -7.98E-1 7.062E3/
318	CH3OCH3+CH3O2=CH3OCH2+CH3O2H	1.68E+13	0	17690	REV/1.544E-6 5.626E0 1.421E4/

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Table B .1. (cont.)

319	CH3OCH3+CH3=CH3OCH2+CH4	1.45E-06	5.73	5700	REV/2.518E11 -6.0E-3 - 2.806E3/
320	CH3OCH3+O2=CH3OCH2+HO2	4.10E+13	0	44910	REV/7.383E10 -2.7E-1 1.026E4/
321	CH3OCH3+CH3O=CH3OCH2+CH3OH	6.02E+11	0	4074	REV/6.428E13 -7.94E-1 7.258E3/
322	CH3OCH3+CH3OCH2O2=CH3OCH2+CH3OCH2O2H	5.00E+12	0	17690	REV/1.723E6 1.746E0 5.832E3/
323	CH3OCH3+O2CHO=CH3OCH2+HO2CHO	4.43E+04	2.6	13910	REV/7.195E12 -3.14E-1 3.313E4/
324	CH3OCH3+OCHO=CH3OCH2+HOCHO	1.00E+13	0	17690	REV/2.601E5 1.879E0 1.667E4/
325	CH3OCH2=CH2O+CH3	1.60E+13	0	25500	REV/1.25E14 3.2E-1 7.854E4/
326	CH3OCH2+CH3O=CH3OCH3+CH2O	2.41E+13	0	0	REV/2.768E4 2.745E0 1.408E4/
327	CH3OCH2+CH2O=CH3OCH3+HCO	5.49E+03	2.8	5862	REV/7.746E11 2.8E-1 1.698E4/
328	CH3OCH2+CH3CHO=CH3OCH3+CH3CO	1.26E+12	0	8499	REV/2.0E12 0.0E0 0.0E0/
329	CH3OCH2O2=CH3OCH2+O2	4.44E+19	-1.594	36240	REV/6.482E13 -8.49E-1 9.455E3/
330	CH3OCH2O2+CH2O=CH3OCH2O2H+HCO	1.00E+12	0	11660	REV/1.0E12 0.0E0 1.0E4/
331	CH3OCH2O2+CH3CHO=CH3OCH2O2H+CH3CO	2.80E+12	0	13600	
332	2CH3OCH2O2=>O2+2CH3OCH2O	2.21E+23	-4.5	0	REV/2.0E13 0.0E0 0.0E0/
333	CH3OCH2O2H=CH3OCH2O+OH	2.11E+22	-2.124	43830	REV/1.0E11 0.0E0 1.19E4/
334	CH3OCH2O=CH3O+CH2O	4.38E+19	-2.014	25190	REV/1.086E10 -2.0E-2 4.648E4/
335	CH3OCH2O+O2=CH3OCHO+HO2	5.00E+10	0	500	REV/1.0E13 0.0E0 7.838E3/
336	CH3OCH2O=CH3OCHO+H	6.06E+12	0.056	8218	REV/1.248E12 -7.65E-1 1.112E4/
337	CH3OCH2O2=CH2OCH2O2H	6.00E+10	0	21580	
338	CH2OCH2O2H=>OH+2CH2O	1.50E+13	0	20760	REV/7.0E11 0.0E0 0.0E0/
339	O2CH2OCH2O2H=CH2OCH2O2H+O2	1.92E+19	-1.622	36270	REV/5.041E3 1.416E0 5.964E4/
340	O2CH2OCH2O2H=HO2CH2OCHO+OH	4.00E+10	0	18580	REV/1.183E8 1.934E0 - 3.952E3/
341	HO2CH2OCHO=OCH2OCHO+OH	2.00E+16	0	40500	REV/1.25E11 0.0E0 1.19E4/
342	OCH2OCHO=CH2O+OCHO	2.90E+19	-2.201	31850	REV/1.568E9 4.87E-1 2.067E4/
343	OCH2OCHO=HOCH2OCO	1.00E+11	0	14000	REV/1.5E11 0.0E0 4.8E3/
344	HOCH2OCO=HOCH2O+CO	2.24E+19	-2.021	19690	REV/1.5E11 0.0E0 3.572E4/
345	HOCH2OCO=CH2OH+CO2	2.41E+17	-1.574	22120	REV/1.0E14 0.0E0 0.0E0/
346	CH3OCHO=CH2OCHO+H	8.24E+19	-1.15	102500	REV/1.0E14 0.0E0 0.0E0/
347	CH3OCHO=CH3OCO+H	1.33E+19	-1	100100	LOW/6.143E60 -1.207E1 7.54E4/ TROE/7.8E-1 8.28E9 4.389E2 6.7E8/
348	CH3OCHO(+M)=CH3OH+CO(+M)	1.00E+14	0	62500	REV/3.0E13 0.0E0 0.0E0/
349	CH3OCHO=CH3O+HCO	5.37E+16	-0.01	97090	REV/1.0E13 0.0E0 0.0E0/
350	CH3OCHO=CH3+OCHO	3.21E+17	-0.53	79970	REV/2.979E10 3.29E-1 9.998E-1/
351	CH3OCHO+O2=CH3OCO+HO2	1.00E+13	0	49700	REV/2.143E10 3.56E-1 3.31E2/
352	CH3OCHO+O2=CH2OCHO+HO2	2.05E+13	0	52000	REV/9.519E4 2.371E0 2.082E4/
353	CH3OCHO+OH=CH3OCO+H2O	1.58E+07	1.8	934	REV/1.114E7 1.568E0 1.95E4/
354	CH3OCHO+OH=CH2OCHO+H2O	5.27E+09	0.97	1586	REV/1.585E3 2.581E0 2.899E3/
355	CH3OCHO+HO2=CH3OCO+H2O2	4.82E+03	2.6	13910	REV/2.746E3 2.558E0 3.513E3/
356	CH3OCHO+HO2=CH2OCHO+H2O2	2.38E+04	2.55	16490	REV/8.126E1 3.108E0 6.408E3/
357	CH3OCHO+O=CH3OCO+OH	2.76E+05	2.45	2830	REV/1.014E2 3.115E0 6.358E3/

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Table B .1. (cont.)

358	CH3OCHO+O=CH2OCHO+OH	9.80E+05	2.43	4750	REV/3.693E2 3.076E0 9.461E3/
359	CH3OCHO+H=CH3OCO+H2	6.50E+05	2.4	4471	REV/1.326E2 3.243E0 9.776E3/
360	CH3OCHO+H=CH2OCHO+H2	6.65E+05	2.54	6756	REV/3.914E-1 3.691E0 1.201E4/
361	CH3OCHO+CH3=CH3OCO+CH4	7.55E-01	3.46	5481	REV/8.222E-2 3.908E0 1.171E4/
362	CH3OCHO+CH3=CH2OCHO+CH4	4.52E-01	3.65	7154	REV/6.685E9 4.64E-1 1.022E4/
363	CH3OCHO+CH3O=CH3OCO+CH3OH	5.48E+11	0	5000	REV/9.289E8 4.91E-1 9.705E3/
364	CH3OCHO+CH3O=CH2OCHO+CH3OH	2.17E+11	0	6458	REV/3.083E4 2.137E0 1.304E3/
365	CH3OCHO+CH3O2=CH3OCO+CH3O2H	4.82E+03	2.6	13910	REV/5.342E4 2.114E0 1.918E3/
366	CH3OCHO+CH3O2=CH2OCHO+CH3O2H	2.38E+04	2.55	16490	REV/5.196E5 2.29E0 6.806E3/
367	CH3OCHO+HCO=CH3OCO+CH2O	5.40E+06	1.9	17010	REV/3.461E3 2.917E0 6.261E3/
368	CH3OCHO+HCO=CH2OCHO+CH2O	1.03E+05	2.5	18430	REV/1.629E12 -1.8E-1 4.067E4/
369	CH2OCHO=CH3OCO	2.62E+11	-0.03	38180	REV/4.76E7 1.54E0 3.47E4/
370	CH3OCO=CH3+CO2	3.59E+14	-0.172	16010	REV/1.55E6 2.02E0 5.73E3/
371	CH3OCO=CH3O+CO	1.43E+15	-0.041	23770	REV/1.5E11 0.0E0 1.19E4/
372	CH2OCHO=CH2O+HCO	4.66E+12	0.12	27440	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/5.64E74 -1.574E1 9.8714E4/ TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
373	C3H8(+M)=CH3+C2H5(+M)	1.29E+37	-5.84	97380	REV/1.0E14 0.0E0 0.0E0/
374	C3H8=NC3H7+H	3.75E+17	-0.357	101200	REV/1.0E14 0.0E0 0.0E0/
375	C3H8=IC3H7+H	2.38E+18	-0.671	98680	REV/1.764E9 5.99E-1 -1.69E2/
376	C3H8+O2=IC3H7+HO2	2.00E+13	0	49640	REV/3.354E10 2.85E-1 -5.9E1/
377	C3H8+O2=NC3H7+HO2	6.00E+13	0	52290	REV/2.186E1 3.347E0 9.351E3/
378	H+C3H8=H2+IC3H7	1.30E+06	2.4	4471	REV/1.418E2 3.173E0 9.096E3/
379	H+C3H8=H2+NC3H7	1.33E+06	2.54	6756	REV/4.793E0 3.428E0 6.608E3/
380	C3H8+O=IC3H7+OH	5.49E+05	2.5	3140	REV/2.053E2 3.014E0 6.433E3/
381	C3H8+O=NC3H7+OH	3.71E+06	2.4	5505	REV/1.191E7 1.497E0 1.882E4/
382	C3H8+OH=NC3H7+H2O	1.05E+10	0.97	1586	REV/8.327E3 2.451E0 1.974E4/
383	C3H8+OH=IC3H7+H2O	4.67E+07	1.61	-35	REV/5.721E2 2.752E0 3.742E3/
384	C3H8+HO2=IC3H7+H2O2	5.88E+04	2.5	14860	REV/4.995E3 2.438E0 3.03E3/
385	C3H8+HO2=NC3H7+H2O2	8.10E+04	2.5	16690	REV/9.819E2 2.671E0 1.394E4/
386	CH3+C3H8=CH4+IC3H7	6.40E+04	2.17	7520	REV/8.791E-2 3.837E0 1.103E4/
387	CH3+C3H8=CH4+NC3H7	9.04E-01	3.65	7154	REV/3.0E10 0.0E0 1.29E4/
388	IC3H7+C3H8=NC3H7+C3H8	3.00E+10	0	12900	REV/1.31E11 0.0E0 1.78E4/
389	C2H3+C3H8=C2H4+IC3H7	1.00E+11	0	10400	REV/1.31E11 0.0E0 1.78E4/
390	C2H3+C3H8=C2H4+NC3H7	1.00E+11	0	10400	REV/3.63E10 0.0E0 9.934E3/
391	C2H5+C3H8=C2H6+IC3H7	1.00E+11	0	10400	REV/3.63E10 0.0E0 9.934E3/

(cont. on next page)

Table B .1. (cont.)

392	C2H5+C3H8=C2H6+NC3H7	1.00E+11	0	10400	REV/5.372E16 -1.33E0 1.34E4/
393	C3H8+C3H5-A=NC3H7+C3H6	7.94E+11	0	20500	REV/5.372E16 -1.33E0 9.095E3/
394	C3H8+C3H5-A=IC3H7+C3H6	7.94E+11	0	16200	REV/1.22E10 0.0E0 9.182E3/
395	C3H8+CH3O=NC3H7+CH3OH	3.00E+11	0	7000	REV/1.22E10 0.0E0 9.182E3/
396	C3H8+CH3O=IC3H7+CH3OH	3.00E+11	0	7000	REV/9.718E4 1.993E0 1.435E3/
397	CH3O2+C3H8=CH3O2H+NC3H7	8.10E+04	2.5	16690	REV/1.113E4 2.307E0 2.147E3/
398	CH3O2+C3H8=CH3O2H+IC3H7	5.88E+04	2.5	14860	REV/9.735E4 1.993E0 1.439E3/
399	C2H5O2+C3H8=C2H5O2H+NC3H7	8.10E+04	2.5	16690	REV/1.115E4 2.307E0 2.151E3/
400	C2H5O2+C3H8=C2H5O2H+IC3H7	5.88E+04	2.5	14860	REV/2.086E13 -5.1E-1 5.0E3/
401	NC3H7O2+C3H8=NC3H7O2H+NC3H7	1.70E+13	0	20460	REV/3.871E11 -1.96E-1 4.08E3/
402	NC3H7O2+C3H8=NC3H7O2H+IC3H7	2.00E+12	0	17000	REV/2.093E13 -5.11E-1 5.0E3/
403	IC3H7O2+C3H8=IC3H7O2H+NC3H7	1.70E+13	0	20460	REV/3.885E11 -1.97E-1 4.08E3/
404	IC3H7O2+C3H8=IC3H7O2H+IC3H7	2.00E+12	0	17000	REV/3.104E10 3.05E-1 8.65E3/
405	C3H8+CH3CO3=IC3H7+CH3CO3H	2.00E+12	0	17000	REV/1.673E12 -9.0E-3 9.57E3/
406	C3H8+CH3CO3=NC3H7+CH3CO3H	1.70E+13	0	20460	REV/1.187E-8 5.54E0 -1.92E3/
407	C3H8+O2CHO=NC3H7+HO2CHO	5.52E+04	2.55	16480	REV/7.838E-6 4.65E0 -3.0E1/
408	C3H8+O2CHO=IC3H7+HO2CHO	1.48E+04	2.6	13910	REV/2.64E13 0.0E0 2.16E3/
409	IC3H7=H+C3H6	6.92E+13	-0.025	37690	REV/4.344E7 1.176E0 8.62E3/
410	IC3H7+H=C2H5+CH3	2.00E+13	0	0	REV/2.0E-19 0.0E0 1.75E4/
411	IC3H7+O2=C3H6+HO2	4.50E-19	0	5020	REV/2.985E12 5.7E-1 8.382E4/
412	IC3H7+OH=C3H6+H2O	2.41E+13	0	0	REV/1.293E16 -1.9E-1 7.938E4/
413	IC3H7+O=CH3COCH3+H	4.82E+13	0	0	REV/1.279E11 8.0E-1 8.648E4/
414	IC3H7+O=CH3CHO+CH3	4.82E+13	0	0	REV/1.898E34 -6.99E0 1.71E4/
415	NC3H7=CH3+C2H4	9.97E+40	-8.6	41430	REV/2.07E37 -7.39E0 1.202E4/
416	NC3H7=H+C3H6	8.78E+39	-8.1	46580	REV/2.0E-19 0.0E0 1.75E4/
417	NC3H7+O2=C3H6+HO2	3.00E-19	0	3000	REV/1.9E14 0.0E0 1.879E4/
418	C2H5CHO+NC3H7=C2H5CO+C3H8	1.70E+12	0	8440	REV/1.9E14 0.0E0 1.879E4/
419	C2H5CHO+IC3H7=C2H5CO+C3H8	1.70E+12	0	8440	REV/1.0E13 0.0E0 2.8E4/
420	C2H5CHO+C3H5-A=C2H5CO+C3H6	1.70E+12	0	8440	REV/6.822E53 -1.1779E1 2.055E4/
421	C3H6=C2H3+CH3	2.73E+62	-13.28	123200	REV/2.041E61 -1.352E1 3.061E4/
422	C3H6=C3H5-A+H	2.01E+61	-13.26	118500	REV/2.551E67 -1.5867E1 2.869E4/
423	C3H6=C3H5-S+H	7.71E+69	-16.09	140000	REV/4.26E68 -1.6164E1 3.008E4/
424	C3H6=C3H5-T+H	5.62E+71	-16.58	139300	REV/9.188E1 2.725E0 2.311E4/
425	C3H6+O=C2H5+HCO	1.58E+07	1.76	-1216	
426	C3H6+O=>CH2CO+CH3+H	2.50E+07	1.76	76	
427	C3H6+O=>CH3CHCO+2H	2.50E+07	1.76	76	REV/1.104E11 6.97E-1 2.015E4/
428	C3H6+O=C3H5-A+OH	5.24E+11	0.7	5884	REV/8.239E7 1.18E0 -2.07E2/
429	C3H6+O=C3H5-S+OH	1.20E+11	0.7	8959	REV/9.483E6 1.373E0 5.76E2/

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Table B .1. (cont.)

430	C3H6+O=C3H5-T+OH	6.03E+10	0.7	7632	REV/1.343E7 1.909E0 3.027E4/
431	C3H6+OH=C3H5-A+H2O	3.12E+06	2	-298	REV/2.959E4 2.393E0 9.916E3/
432	C3H6+OH=C3H5-S+H2O	2.11E+06	2	2778	REV/3.565E3 2.586E0 1.07E4/
433	C3H6+OH=C3H5-T+H2O	1.11E+06	2	1451	REV/6.341E6 1.82E0 1.201E4/
434	C3H6+HO2=C3H5-A+H2O2	2.70E+04	2.5	12340	REV/1.377E4 2.304E0 3.864E3/
435	C3H6+HO2=C3H5-S+H2O2	1.80E+04	2.5	27620	REV/1.577E3 2.497E0 1.941E3/
436	C3H6+HO2=C3H5-T+H2O2	9.00E+03	2.5	23590	REV/7.023E4 2.515E0 1.817E4/
437	C3H6+H=C3H5-A+H2	1.73E+05	2.5	2492	REV/1.063E3 2.999E0 4.526E3/
438	C3H6+H=C3H5-S+H2	8.04E+05	2.5	12280	REV/1.227E2 3.192E0 4.15E3/
439	C3H6+H=C3H5-T+H2	4.05E+05	2.5	9794	REV/7.272E7 1.271E0 1.12E4/
440	C3H6+H=C2H4+CH3	2.30E+13	0	2547	REV/8.514E12 -3.33E-1 8.87E2/
441	C3H6+O2=C3H5-A+HO2	4.00E+12	0	39900	REV/1.387E10 1.51E-1 4.59E2/
442	C3H6+O2=C3H5-S+HO2	2.00E+12	0	62900	REV/2.224E9 3.44E-1 3.69E2/
443	C3H6+O2=C3H5-T+HO2	1.40E+12	0	60700	REV/8.184E2 3.07E0 2.289E4/
444	C3H6+CH3=C3H5-A+CH4	2.21E+00	3.5	5675	REV/1.626E0 3.553E0 6.635E3/
445	C3H6+CH3=C3H5-S+CH4	1.35E+00	3.5	12850	REV/2.322E-1 3.746E0 7.552E3/
446	C3H6+CH3=C3H5-T+CH4	8.40E-01	3.5	11660	REV/5.369E5 1.33E0 1.644E4/
447	C3H6+C2H5=C3H5-A+C2H6	1.00E+11	0	9800	REV/2.0E10 0.0E0 1.5E4/
448	C3H6+CH3CO3=C3H5-A+CH3CO3H	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
449	C3H6+CH3O2=C3H5-A+CH3O2H	3.24E+11	0	14900	REV/1.0E-10 0.0E0 0.0E0/
450	C3H6+HO2=C3H6O1-2+OH	1.29E+12	0	14900	REV/2.0E10 0.0E0 1.5E4/
451	C3H6+C2H5O2=C3H5-A+C2H5O2H	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
452	C3H6+NC3H7O2=C3H5-A+NC3H7O2H	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
453	C3H6+IC3H7O2=C3H5-A+IC3H7O2H	3.24E+11	0	14900	REV/9.93E11 0.0E0 -9.6E2/
454	C3H6OH=C3H6+OH	4.34E+15	-0.805	27900	REV/1.2E11 0.0E0 -1.1E3/
455	HOC3H6O2=C3H6OH+O2	2.87E+19	-1.897	34290	
456	HOC3H6O2=>CH3CHO+CH2O+OH	1.25E+10	0	18900	REV/2.61E46 -9.82E0 3.695E4/
457	C3H5-A=C2H2+CH3	2.40E+48	-9.9	82080	REV/2.4E11 6.9E-1 3.007E3/
458	C3H5-A=C3H4-A+H	4.19E+13	0.216	61930	REV/1.605E12 6.0E-2 1.166E4/
459	C3H5-A+HO2=C3H5O+OH	7.00E+12	0	-1000	REV/1.99E15 -7.4E-1 1.702E4/
460	C3H5-A+CH3O2=C3H5O+CH3O	7.00E+12	0	-1000	REV/1.802E12 5.0E-2 4.033E4/
461	C3H5-A+C2H5=C2H6+C3H4-A	4.00E+11	0	0	REV/6.937E16 -1.33E0 5.28E4/
462	C3H5-A+C2H5=C2H4+C3H6	4.00E+11	0	0	REV/1.624E13 5.0E-2 4.819E4/
463	C3H5-A+C2H3=C2H4+C3H4-A	1.00E+12	0	0	REV/8.43E10 0.0E0 -2.62E2/
464	C3H4-A+C3H6=2C3H5-A	4.75E+08	0.734	28700	REV/2.614E19 -2.449E0 2.071E4/
465	C3H5-A+O2=C3H4-A+HO2	2.18E+21	-2.85	30760	REV/4.944E16 -1.4E0 8.862E4/
466	C3H5-A+O2=CH2CHO+CH2O	7.14E+15	-1.21	21050	REV/1.989E13 -6.09E-1 7.514E4/
467	C3H5-A+O2=C2H3CHO+OH	2.47E+13	-0.44	23020	

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Table B .1. (cont.)

468	C3H5-A+O2=>C2H2+CH2O+OH	9.72E+29	-5.71	21450	REV/1.61E40 -8.58E0 2.033E4/
469	C3H5-S=C2H2+CH3	9.60E+39	-8.17	42030	REV/5.8E12 0.0E0 3.1E3/
470	C3H5-S=C3H4-P+H	4.19E+15	-0.79	37480	REV/1.611E17 -1.27E0 9.653E4/
471	C3H5-S+O2=CH3CHO+HCO	4.34E+12	0	0	REV/7.977E12 1.1E-1 6.886E4/
472	C3H5-S+H=C3H4-A+H2	3.33E+12	0	0	REV/6.253E12 1.1E-1 6.934E4/
473	C3H5-S+CH3=C3H4-A+CH4	1.00E+11	0	0	REV/1.61E40 -8.58E0 2.033E4/
474	C3H5-T=C2H2+CH3	2.16E+40	-8.31	45110	REV/8.5E12 0.0E0 2.0E3/
475	C3H5-T=C3H4-A+H	3.51E+14	-0.44	40890	REV/6.5E12 0.0E0 2.0E3/
476	C3H5-T=C3H4-P+H	1.08E+15	-0.6	38490	REV/3.037E31 -5.865E0 2.681E4/
477	C3H5-T+O2=C3H4-A+HO2	1.89E+30	-5.59	15540	REV/2.0E11 0.0E0 1.75E4/
478	C3H5-T+O2=CH3COCH2+O	3.81E+17	-1.36	5580	REV/1.872E27 -4.43E0 1.012E5/
479	C3H5-T+O2=CH2O+CH3CO	3.71E+25	-3.96	7043	REV/2.138E16 -8.8E-1 7.105E4/
480	C3H5-T+H=C3H4-P+H2	3.33E+12	0	0	REV/1.676E16 -8.8E-1 7.153E4/
481	C3H5-T+CH3=C3H4-P+CH4	1.00E+11	0	0	REV/3.222E18 -9.9E-1 9.659E4/
482	C3H4-A=C3H4-P	1.20E+15	0	92400	REV/3.17E11 -8.6E-2 3.11E2/
483	C3H4-A+O2=C3H3+HO2	4.00E+13	0	39160	REV/1.0E0 0.0E0 0.0E0/
484	C3H4-A+HO2=CH2CO+CH2+OH	4.00E+12	0	19000	REV/1.806E17 -1.38E0 3.607E4/
485	C3H4-A+OH=CH2CO+CH3	3.12E+12	0	-397	REV/3.269E8 1.252E0 1.219E5/
486	C3H4-A+O=C2H4+CO	7.80E+12	0	1600	REV/2.32E2 3.23E0 8.119E4/
487	C3H4-A+O=C2H2+CH2O	3.00E-03	4.61	-4243	REV/2.644E19 -2.71E0 4.214E4/
488	C3H4-A+C3H5-A=C3H3+C3H6	2.00E+11	0	7700	REV/1.42E16 -1.38E0 5.382E4/
489	C3H4-A+C2H=C3H3+C2H2	1.00E+13	0	0	REV/1.0E0 0.0E0 0.0E0/
490	C3H4-P+O2=HCCO+OH+CH2	1.00E+07	1.5	30100	REV/6.371E11 -2.08E-1 1.021E3/
491	C3H4-P+O2=C3H3+HO2	2.00E+13	0	41600	REV/1.0E0 0.0E0 0.0E0/
492	C3H4-P+HO2=C2H4+CO+OH	3.00E+12	0	19000	REV/6.441E5 2.034E0 3.0E4/
493	C3H4-P+OH=C3H3+H2O	1.00E+07	2	1000	REV/1.079E-2 4.11E0 3.128E4/
494	C3H4-P+OH=CH2CO+CH3	5.00E-04	4.5	-1000	REV/2.548E12 -3.9E-1 3.235E4/
495	C3H4-P+O=C2H3+HCO	3.20E+12	0	2010	REV/1.43E4 1.793E0 2.699E4/
496	C3H4-P+O=HCCO+CH3	9.60E+08	1	0	REV/1.0E-30 0.0E0 0.0E0/
497	C3H4-P+O=HCCO+CH2+H	3.20E-19	0	2010	REV/2.177E8 1.31E0 2.247E4/
498	C3H4-P+O=C3H3+OH	7.65E+08	1.5	8600	REV/1.215E5 2.14E0 1.911E4/
499	C3H4-P+H=C3H3+H2	2.00E+07	2	5000	REV/8.313E0 3.195E0 2.125E4/
500	C3H4-P+CH3=C3H3+CH4	1.50E+00	3.5	5600	REV/9.541E11 -3.9E-1 5.245E4/
501	C3H4-P+C2H3=C3H3+C2H4	1.00E+12	0	7700	REV/4.931E16 -1.73E0 3.795E4/
502	C3H4-P+C3H5-A=C3H3+C3H6	1.00E+12	0	7700	
503	C3H3+OH=C3H2+H2O	2.00E+13	0	8000	REV/4.881E11 0.0E0 5.947E4/
504	C3H3+O2=CH2CO+HCO	3.01E+10	0	2870	REV/1.81E13 0.0E0 0.0E0/
505	C3H3+CH3=C2H5+C2H	4.30E+15	-0.79	45630	REV/2.326E14 -2.14E-1 7.719E4/

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Table B .1. (cont.)

506	C3H2+O2=HCO+HCCO	5.00E+13	0	0	REV/1.0E0 0.0E0 0.0E0/
507	C3H4-A+HO2=C2H4+CO+OH	1.00E+12	0	14000	REV/1.551E16 -1.38E0 4.4E4/
508	C3H4-A+HO2=C3H3+H2O2	3.00E+13	0	14000	REV/6.407E25 -3.345E0 2.177E4/
509	C2H2+CH3=C3H4-A+H	6.74E+19	-2.08	31590	
510	C3H3+H=C3H2+H2	2.14E+05	2.52	7453	REV/2.282E16 -2.54E-1 7.502E4/
511	C3H2+OH=C2H2+HCO	5.00E+13	0	0	
512	C3H2+O2=>HCCO+CO+H	5.00E+13	0	0	
513	CH3CHCO+OH=>C2H5+CO2	1.73E+12	0	-1010	
514	CH3CHCO+OH=>SC2H4OH+CO	2.00E+12	0	-1010	
515	CH3CHCO+H=>C2H5+CO	4.40E+12	0	1459	
516	CH3CHCO+O=>CH3CHO+CO	3.20E+12	0	-437	REV/6.22E15 -6.92E-1 2.531E4/
517	NC3H7+HO2=NC3H7O+OH	7.00E+12	0	-1000	REV/1.051E16 -5.57E-1 2.732E4/
518	IC3H7+HO2=IC3H7O+OH	7.00E+12	0	-1000	REV/3.89E14 -3.94E-1 2.955E4/
519	CH3O2+NC3H7=CH3O+NC3H7O	7.00E+12	0	-1000	REV/6.573E14 -2.58E-1 3.156E4/
520	CH3O2+IC3H7=CH3O+IC3H7O	7.00E+12	0	-1000	REV/4.52E12 0.0E0 0.0E0/
521	NC3H7O2=NC3H7+O2	2.40E+20	-1.616	35960	REV/7.54E12 0.0E0 0.0E0/
522	IC3H7O2=IC3H7+O2	3.13E+22	-2.167	38160	REV/8.0E11 0.0E0 1.0E4/
523	NC3H7O2+CH2O=NC3H7O2H+HCO	5.60E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
524	NC3H7O2+CH3CHO=NC3H7O2H+CH3CO	2.80E+12	0	13600	REV/8.0E11 0.0E0 1.0E4/
525	IC3H7O2+CH2O=IC3H7O2H+HCO	5.60E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
526	IC3H7O2+CH3CHO=IC3H7O2H+CH3CO	2.80E+12	0	13600	REV/3.841E13 -7.95E-1 3.361E4/
527	NC3H7O2+HO2=NC3H7O2H+O2	1.75E+10	0	-3275	REV/3.855E13 -7.96E-1 3.361E4/
528	IC3H7O2+HO2=IC3H7O2H+O2	1.75E+10	0	-3275	REV/3.0E12 0.0E0 1.15E4/
529	C2H4+NC3H7O2=C2H3+NC3H7O2H	1.13E+13	0	30430	REV/3.0E12 0.0E0 1.15E4/
530	C2H4+IC3H7O2=C2H3+IC3H7O2H	1.13E+13	0	30430	REV/1.0E9 0.0E0 1.0E4/
531	CH3OH+NC3H7O2=CH2OH+NC3H7O2H	6.30E+12	0	19360	REV/1.0E9 0.0E0 1.0E4/
532	CH3OH+IC3H7O2=CH2OH+IC3H7O2H	6.30E+12	0	19360	REV/1.0E12 0.0E0 1.0E4/
533	C2H3CHO+NC3H7O2=C2H3CO+NC3H7O2H	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
534	C2H3CHO+IC3H7O2=C2H3CO+IC3H7O2H	2.80E+12	0	13600	REV/7.43E11 0.0E0 5.5E3/
535	CH4+NC3H7O2=CH3+NC3H7O2H	1.12E+13	0	24640	REV/7.43E11 0.0E0 5.5E3/
536	CH4+IC3H7O2=CH3+IC3H7O2H	1.12E+13	0	24640	
537	NC3H7O2+CH3O2=>NC3H7O+CH3O+O2	1.40E+16	-1.61	1860	
538	IC3H7O2+CH3O2=>IC3H7O+CH3O+O2	1.40E+16	-1.61	1860	REV/4.8E13 0.0E0 7.95E3/
539	H2+NC3H7O2=H+NC3H7O2H	3.01E+13	0	26030	REV/4.8E13 0.0E0 7.95E3/
540	H2+IC3H7O2=H+IC3H7O2H	3.01E+13	0	26030	REV/5.0E11 0.0E0 6.5E3/
541	IC3H7O2+C2H6=IC3H7O2H+C2H5	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
542	NC3H7O2+C2H6=NC3H7O2H+C2H5	1.70E+13	0	20460	REV/5.0E9 0.0E0 1.0E4/
543	IC3H7O2+C2H5CHO=IC3H7O2H+C2H5CO	2.00E+11	0	9500	REV/5.0E9 0.0E0 1.0E4/
544	NC3H7O2+C2H5CHO=NC3H7O2H+C2H5CO	2.00E+11	0	9500	
545	IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2	1.40E+16	-1.61	1860	
546	NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2	1.40E+16	-1.61	1860	
547	IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2	1.40E+16	-1.61	1860	
548	NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2	1.40E+16	-1.61	1860	
549	2IC3H7O2=>O2+2IC3H7O	1.40E+16	-1.61	1860	
550	2NC3H7O2=>O2+2NC3H7O	1.40E+16	-1.61	1860	

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Table B .1. (cont.)

551	IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2	1.40E+16	-1.61	1860	REV/1.145E11 6.95E-1 2.672E4/
552	IC3H7O2+CH3=IC3H7O+CH3O	7.00E+12	0	-1000	REV/1.628E13 9.4E-2 2.913E4/
553	IC3H7O2+C2H5=IC3H7O+C2H5O	7.00E+12	0	-1000	REV/2.778E13 2.61E-1 2.98E4/
554	IC3H7O2+IC3H7=2IC3H7O	7.00E+12	0	-1000	REV/1.644E13 1.25E-1 2.78E4/
555	IC3H7O2+NC3H7=IC3H7O+NC3H7O	7.00E+12	0	-1000	REV/4.242E9 8.77E-1 1.414E4/
556	IC3H7O2+C3H5-A=IC3H7O+C3H5O	7.00E+12	0	-1000	REV/5.303E12 9.0E-3 2.692E4/
557	NC3H7O2+CH3=NC3H7O+CH3O	7.00E+12	0	-1000	REV/7.54E14 -5.92E-1 2.933E4/
558	NC3H7O2+C2H5=NC3H7O+C2H5O	7.00E+12	0	-1000	REV/1.286E15 -4.25E-1 3.0E4/
559	NC3H7O2+IC3H7=NC3H7O+IC3H7O	7.00E+12	0	-1000	REV/7.612E14 -5.61E-1 2.8E4/
560	NC3H7O2+NC3H7=2NC3H7O	7.00E+12	0	-1000	REV/1.964E11 1.91E-1 1.434E4/
561	NC3H7O2+C3H5-A=NC3H7O+C3H5O	7.00E+12	0	-1000	REV/1.143E8 1.719E0 -4.034E3/
562	NC3H7O2H=NC3H7O+OH	1.50E+16	0	42500	REV/1.55E6 2.406E0 -4.132E3/
563	IC3H7O2H=IC3H7O+OH	9.45E+15	0	42600	REV/1.0E11 0.0E0 3.496E3/
564	NC3H7O=C2H5+CH2O	2.72E+21	-2.449	15700	REV/4.0E12 0.0E0 6.26E3/
565	NC3H7O=C2H5CHO+H	8.90E+10	0.746	19800	REV/1.0E11 0.0E0 9.256E3/
566	IC3H7O=CH3+CH3CHO	5.33E+19	-1.696	17140	REV/2.0E12 0.0E0 7.27E3/
567	IC3H7O=CH3COCH3+H	8.66E+14	-0.483	20080	REV/1.0E11 0.0E0 3.2E4/
568	IC3H7O+O2=CH3COCH3+HO2	9.09E+09	0	390	REV/1.117E8 5.83E-1 1.172E4/
569	NC3H7O2=C3H6OOH1-2	6.00E+11	0	26850	REV/2.716E11 -5.07E-1 8.936E3/
570	NC3H7O2=C3H6OOH1-3	1.13E+11	0	24400	REV/1.122E10 1.19E-1 1.181E4/
571	IC3H7O2=C3H6OOH2-1	1.80E+12	0	29400	REV/2.384E34 -7.06E0 4.494E4/
572	IC3H7O2=C3H6OOH2-2	1.23E+35	-6.96	48880	REV/1.15E11 4.9E-1 3.837E4/
573	C3H6OOH1-2=C3H6O1-2+OH	6.00E+11	0	22000	REV/1.186E6 1.765E0 2.871E4/
574	C3H6OOH1-3=C3H6O1-3+OH	7.50E+10	0	15250	REV/2.78E8 1.191E0 3.609E4/
575	C3H6OOH2-1=C3H6O1-2+OH	6.00E+11	0	22000	REV/1.0E11 0.0E0 1.1E4/
576	C3H6OOH1-2=C3H6+HO2	7.83E+15	-1.3	15950	REV/1.0E11 0.0E0 1.175E4/
577	C3H6OOH2-1=C3H6+HO2	3.24E+18	-2	18970	
578	C3H6OOH1-3=>OH+CH2O+C2H4	3.04E+15	-0.79	27400	REV/4.46E22 -4.24E0 1.063E4/
579	C3H6OOH2-1=C2H3OOH+CH3	6.54E+27	-5.14	38320	
580	C3H6OOH1-2=>C2H4+CH2O+OH	1.31E+33	-7.01	48120	REV/1.021E14 3.1E-1 3.675E4/
581	C3H6OOH2-2=CH3COCH3+OH	9.00E+14	0	1500	REV/5.0E12 0.0E0 0.0E0/
582	C3H6OOH1-2O2=C3H6OOH1-2+O2	2.39E+25	-2.945	40100	REV/4.52E12 0.0E0 0.0E0/
583	C3H6OOH1-3O2=C3H6OOH1-3+O2	2.85E+20	-1.626	35690	REV/4.52E12 0.0E0 0.0E0/
584	C3H6OOH2-1O2=C3H6OOH2-1+O2	5.23E+22	-2.244	37820	REV/9.249E4 1.329E0 4.892E4/
585	C3H6OOH1-2O2=C3KET12+OH	6.00E+11	0	26400	REV/4.101E3 1.496E0 4.474E4/
586	C3H6OOH1-3O2=C3KET13+OH	7.50E+10	0	21400	REV/1.397E3 1.834E0 4.975E4/
587	C3H6OOH2-1O2=C3KET21+OH	3.00E+11	0	23850	REV/2.391E11 -4.99E-1 8.92E3/
588	C3H6OOH2-1O2=C3H51-2,3OOH	1.13E+11	0	24400	REV/1.913E12 -4.99E-1 1.392E4/
589	C3H6OOH1-2O2=C3H51-2,3OOH	9.00E+11	0	29400	REV/3.18E15 -1.16E0 1.204E4/

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Table B .1. (cont.)

590	C3H51-2,3OOH=AC3H5OOH+HO2	2.56E+13	-0.49	17770	REV/6.0E11 0.0E0 2.685E4/
591	C3H52-1,3OOH=C3H6OOH1-3O2	1.26E+12	-0.36	13940	REV/1.564E11 1.2E-1 1.02E4/
592	C3H52-1,3OOH=AC3H5OOH+HO2	1.15E+14	-0.63	17250	
593	C3KET12=>CH3CHO+HCO+OH	9.45E+15	0	43000	
594	C3KET13=>CH2O+CH2CHO+OH	1.00E+16	0	43000	
595	C3KET21=>CH2O+CH3CO+OH	1.00E+16	0	43000	REV/2.0E13 0.0E0 0.0E0/
596	AC3H5OOH=C3H5O+OH	3.88E+19	-1.46	45370	REV/1.676E14 -1.56E-1 1.969E4/
597	C3H5O=C2H3CHO+H	1.00E+14	0	29100	REV/1.5E11 0.0E0 1.06E4/
598	C3H5O=C2H3+CH2O	1.46E+20	-1.968	35090	REV/1.288E11 0.0E0 3.2E4/
599	C3H5O+O2=C2H3CHO+HO2	1.00E+12	0	6000	REV/1.0E11 0.0E0 0.0E0/
600	C2H3OOH=CH2CHO+OH	8.40E+14	0	43000	REV/2.97E11 1.0E0 3.108E4/
601	C3H6O1-2=C2H4+CH2O	6.00E+14	0	60000	
602	C3H6O1-2+OH=>CH2O+C2H3+H2O	5.00E+12	0	0	
603	C3H6O1-2+H=>CH2O+C2H3+H2	2.63E+07	2	5000	
604	C3H6O1-2+O=>CH2O+C2H3+OH	8.43E+13	0	5200	
605	C3H6O1-2+HO2=>CH2O+C2H3+H2O2	1.00E+13	0	15000	
606	C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H	1.00E+13	0	19000	
607	C3H6O1-2+CH3=>CH2O+C2H3+CH4	2.00E+11	0	10000	REV/2.97E11 0.0E0 3.108E4/
608	C3H6O1-3=C2H4+CH2O	6.00E+14	0	60000	
609	C3H6O1-3+OH=>CH2O+C2H3+H2O	5.00E+12	0	0	
610	C3H6O1-3+O=>CH2O+C2H3+OH	8.43E+13	0	5200	
611	C3H6O1-3+H=>CH2O+C2H3+H2	2.63E+07	2	5000	
612	C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H	1.00E+13	0	19000	
613	C3H6O1-3+HO2=>CH2O+C2H3+H2O2	1.00E+13	0	15000	
614	C3H6O1-3+CH3=>CH2O+C2H3+CH4	2.00E+11	0	10000	REV/1.954E33 -7.289E0 1.667E4/
615	IC3H7O2=C3H6+HO2	1.02E+43	-9.409	41490	REV/1.198E30 -6.229E0 2.042E4/
616	NC3H7O2=C3H6+HO2	5.04E+38	-8.112	40490	LOW/4.72E18 0.0E0 4.9576E4/ TROE/7.2E-1 1.5E3 1.0E-10 1.0E10/
617	C4H10(+M)=2C2H5(+M)	2.72E+15	0	75610	LOW/5.34E17 0.0E0 4.2959E4/ TROE/7.2E-1 1.5E3 1.0E-10 1.0E10/
618	C4H10(+M)=NC3H7+CH3(+M)	4.28E+14	0	69900	REV/3.61E13 0.0E0 0.0E0/
619	C4H10=PC4H9+H	1.34E+17	-0.356	101200	REV/3.61E13 0.0E0 0.0E0/
620	C4H10=SC4H9+H	1.98E+18	-0.694	98720	REV/3.377E10 2.84E-1 -1.9E1/
621	C4H10+O2=PC4H9+HO2	6.00E+13	0	52340	REV/1.532E9 6.22E-1 -4.9E1/
622	C4H10+O2=SC4H9+HO2	4.00E+13	0	49800	REV/1.0E12 0.0E0 2.0E4/
623	C4H10+C3H5-A=PC4H9+C3H6	7.94E+11	0	20500	REV/1.0E12 0.0E0 2.0E4/
624	C4H10+C3H5-A=SC4H9+C3H6	3.16E+11	0	16400	REV/3.56E10 0.0E0 1.292E4/
625	C4H10+C2H5=PC4H9+C2H6	1.58E+11	0	12300	REV/7.12E10 0.0E0 9.917E3/
626	C4H10+C2H5=SC4H9+C2H6	1.00E+11	0	10400	REV/2.57E12 0.0E0 2.538E4/
627	C4H10+C2H3=PC4H9+C2H4	1.00E+12	0	18000	REV/2.05E12 0.0E0 2.418E4/
628	C4H10+C2H3=SC4H9+C2H4	8.00E+11	0	16800	REV/8.853E-2 3.836E0 1.102E4/
629	C4H10+CH3=PC4H9+CH4	9.04E-01	3.65	7154	REV/2.013E-2 3.984E0 1.186E4/
630	C4H10+CH3=SC4H9+CH4	3.02E+00	3.46	5481	REV/2.018E1 3.382E0 8.61E3/

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Table B .1. (cont.)

631	C4H10+H=PC4H9+H2	1.88E+05	2.75	6280	REV/1.9E1 3.37E0 9.311E3/
632	C4H10+H=SC4H9+H2	2.60E+06	2.4	4471	REV/1.2E7 1.496E0 1.881E4/
633	C4H10+OH=PC4H9+H2O	1.05E+10	0.97	1586	REV/7.235E3 2.474E0 1.97E4/
634	C4H10+OH=SC4H9+H2O	9.34E+07	1.61	-35	REV/1.48E13 0.0E0 1.224E4/
635	C4H10+O=PC4H9+OH	1.13E+14	0	7850	REV/7.35E12 0.0E0 9.59E3/
636	C4H10+O=SC4H9+OH	5.62E+13	0	5200	REV/2.534E0 3.527E0 3.49E3/
637	C4H10+HO2=PC4H9+H2O2	4.08E+01	3.59	17160	REV/5.343E-1 3.645E0 2.558E3/
638	C4H10+HO2=SC4H9+H2O2	1.26E+02	3.37	13720	REV/1.22E10 0.0E0 5.0E4/
639	C4H10+CH3O=PC4H9+CH3OH	3.00E+11	0	7000	REV/2.441E10 0.0E0 5.0E4/
640	C4H10+CH3O=SC4H9+CH3OH	6.00E+11	0	7000	REV/1.0E10 0.0E0 9.0E3/
641	C4H10+C2H5O=PC4H9+C2H5OH	3.00E+11	0	7000	REV/1.0E10 0.0E0 9.0E3/
642	C4H10+C2H5O=SC4H9+C2H5OH	6.00E+11	0	7000	REV/1.5E11 0.0E0 1.23E4/
643	C4H10+PC4H9=SC4H9+C4H10	1.00E+11	0	10400	REV/5.0E11 0.0E0 6.5E3/
644	C4H10+CH3CO3=PC4H9+CH3CO3H	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
645	C4H10+CH3CO3=SC4H9+CH3CO3H	1.12E+13	0	17700	REV/3.68E0 2.99E0 2.505E3/
646	C4H10+O2CHO=PC4H9+HO2CHO	1.68E+13	0	20440	REV/7.595E3 2.06E0 4.266E3/
647	C4H10+O2CHO=SC4H9+HO2CHO	1.12E+13	0	17690	REV/1.675E0 3.462E0 3.016E3/
648	CH3O2+C4H10=CH3O2H+PC4H9	1.39E+00	3.97	18280	REV/1.675E0 3.41E0 2.05E3/
649	CH3O2+C4H10=CH3O2H+SC4H9	2.04E+01	3.58	14810	REV/4.938E1 3.082E0 1.899E3/
650	C2H5O2+C4H10=C2H5O2H+PC4H9	4.08E+01	3.59	17160	REV/1.041E1 3.2E0 9.67E2/
651	C2H5O2+C4H10=C2H5O2H+SC4H9	1.26E+02	3.37	13720	REV/5.0E11 0.0E0 6.5E3/
652	NC3H7O2+C4H10=NC3H7O2H+PC4H9	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
653	NC3H7O2+C4H10=NC3H7O2H+SC4H9	1.12E+13	0	17700	REV/5.0E11 0.0E0 6.5E3/
654	IC3H7O2+C4H10=IC3H7O2H+PC4H9	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
655	IC3H7O2+C4H10=IC3H7O2H+SC4H9	1.12E+13	0	17700	REV/5.0E11 0.0E0 6.5E3/
656	PC4H9O2+C3H8=PC4H9O2H+NC3H7	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
657	PC4H9O2+C3H8=PC4H9O2H+IC3H7	2.00E+12	0	17000	REV/5.0E11 0.0E0 6.5E3/
658	PC4H9O2+C4H10=PC4H9O2H+PC4H9	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
659	PC4H9O2+C4H10=PC4H9O2H+SC4H9	1.12E+13	0	17700	REV/5.0E11 0.0E0 6.5E3/
660	SC4H9O2+C3H8=SC4H9O2H+NC3H7	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
661	SC4H9O2+C3H8=SC4H9O2H+IC3H7	2.00E+12	0	17000	REV/5.0E11 0.0E0 6.5E3/
662	SC4H9O2+C4H10=SC4H9O2H+PC4H9	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
663	SC4H9O2+C4H10=SC4H9O2H+SC4H9	1.12E+13	0	17700	REV/1.32E4 2.48E0 6.13E3/
664	PC4H9=C2H5+C2H4	3.50E+12	0.463	29470	REV/1.76E4 2.48E0 6.13E3/
665	SC4H9=C3H6+CH3	4.80E+10	1.044	30350	REV/2.5E11 5.1E-1 2.62E3/
666	PC4H9=C4H8-1+H	2.62E+12	0.253	35700	REV/2.5E11 5.1E-1 2.62E3/
667	SC4H9=C4H8-2+H	2.84E+11	0.337	35520	REV/4.24E11 5.1E-1 1.23E3/
668	SC4H9=C4H8-1+H	3.03E+11	0.591	36820	REV/2.0E-19 0.0E0 1.75E4/
669	PC4H9+O2=C4H8-1+HO2	2.00E-18	0	5000	REV/2.0E-19 0.0E0 1.75E4/
670	SC4H9+O2=C4H8-1+HO2	2.00E-18	0	5000	REV/2.0E-19 0.0E0 1.75E4/
671	SC4H9+O2=C4H8-2+HO2	2.00E-18	0	5000	REV/1.35E13 0.0E0 0.0E0/
672	C4H8-1=C3H5-A+CH3	5.08E+19	-1.256	76510	REV/9.0E12 0.0E0 0.0E0/
673	C4H8-1=C2H3+C2H5	2.88E+23	-1.99	101600	REV/5.0E13 0.0E0 0.0E0/
674	C4H8-1=H+C4H71-3	3.72E+14	-0.111	85200	REV/4.653E12 7.0E-2 -1.68E2/

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Table B .1. (cont.)

675	C4H8-1+O2=C4H71-3+HO2	2.00E+13	0	37190	REV/2.213E5 2.36E0 6.469E3/
676	C4H8-1+H=C4H71-1+H2	7.81E+05	2.5	12290	REV/2.558E4 2.55E0 2.125E3/
677	C4H8-1+H=C4H71-2+H2	3.90E+05	2.5	5821	REV/4.323E6 2.1E0 2.033E4/
678	C4H8-1+H=C4H71-3+H2	3.38E+05	2.36	207	REV/3.045E4 2.54E0 1.103E4/
679	C4H8-1+H=C4H71-4+H2	6.65E+05	2.54	6756	REV/2.625E6 1.86E0 1.212E4/
680	C4H8-1+OH=C4H71-1+H2O	2.14E+06	2	2778	REV/6.304E5 2.05E0 1.291E4/
681	C4H8-1+OH=C4H71-2+H2O	2.22E+06	2	1451	REV/1.532E6 2.38E0 3.336E4/
682	C4H8-1+OH=C4H71-3+H2O	2.76E+04	2.64	-1919	REV/1.044E9 9.7E-1 2.101E4/
683	C4H8-1+OH=C4H71-4+H2O	5.27E+09	0.97	1586	REV/1.234E3 3.05E0 2.461E4/
684	C4H8-1+CH3=C4H71-3+CH4	3.69E+00	3.31	4002	REV/5.405E-1 3.65E0 1.191E4/
685	C4H8-1+CH3=C4H71-4+CH4	4.52E-01	3.65	7154	REV/1.586E6 1.96E0 1.435E4/
686	C4H8-1+HO2=C4H71-3+H2O2	4.82E+03	2.55	10530	REV/2.8E3 2.22E0 4.46E3/
687	C4H8-1+HO2=C4H71-4+H2O2	2.38E+03	2.55	16490	REV/3.303E6 1.79E0 1.133E4/
688	C4H8-1+CH3O2=C4H71-3+CH3O2H	4.82E+03	2.55	10530	REV/5.831E3 2.04E0 1.44E3/
689	C4H8-1+CH3O2=C4H71-4+CH3O2H	2.38E+03	2.55	16490	REV/2.47E2 2.67E0 2.7E4/
690	C4H8-1+CH3O=C4H71-3+CH3OH	4.00E+01	2.9	8609	REV/4.789E9 2.0E-2 9.002E3/
691	C4H8-1+CH3O=C4H71-4+CH3OH	2.17E+11	0	6458	REV/2.0E10 0.0E0 1.0E4/
692	C4H8-1+CH3CO3=C4H71-3+CH3CO3H	1.00E+11	0	8000	REV/1.0E11 0.0E0 1.75E4/
693	C4H8-1+C3H5-A=C4H71-3+C3H6	7.90E+10	0	12400	REV/1.6E12 0.0E0 0.0E0/
694	C4H8-1+C4H6=2C4H71-3	2.35E+12	0	46720	REV/3.16E11 0.0E0 1.3E4/
695	C4H8-1+C2H5O2=C4H71-3+C2H5O2H	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
696	C4H8-1+NC3H7O2=C4H71-3+NC3H7O2H	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
697	C4H8-1+IC3H7O2=C4H71-3+IC3H7O2H	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
698	C4H8-1+PC4H9O2=C4H71-3+PC4H9O2H	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
699	C4H8-1+SC4H9O2=C4H71-3+SC4H9O2H	1.40E+12	0	14900	
700	C4H8-1+CH3O2=>C4H8O1-2+CH3O	1.00E+12	0	14340	REV/5.0E13 0.0E0 0.0E0/
701	C4H8-2=H+C4H71-3	2.34E+14	0.143	87890	REV/1.35E13 -1.8E-1 -9.24E2/
702	C4H8-2+O2=C4H71-3+HO2	4.00E+13	0	39390	REV/6.428E6 1.99E0 1.966E4/
703	C4H8-2+H=C4H71-3+H2	3.46E+05	2.5	2492	REV/5.019E8 1.49E0 3.202E4/
704	C4H8-2+OH=C4H71-3+H2O	6.24E+06	2	-298	REV/2.145E3 2.99E0 2.332E4/
705	C4H8-2+CH3=C4H71-3+CH4	4.42E+00	3.5	5675	REV/9.205E6 1.77E0 1.477E4/
706	C4H8-2+HO2=C4H71-3+H2O2	1.93E+04	2.6	13910	REV/1.917E7 1.59E0 1.175E4/
707	C4H8-2+CH3O2=C4H71-3+CH3O2H	1.93E+04	2.6	13910	REV/1.612E2 2.47E0 2.742E4/
708	C4H8-2+CH3O=C4H71-3+CH3OH	1.80E+01	2.95	11990	REV/1.585E11 0.0E0 1.47E4/
709	C4H8-2+C2H5O2=C4H71-3+C2H5O2H	3.20E+12	0	14900	REV/1.585E11 0.0E0 1.47E4/
710	C4H8-2+NC3H7O2=C4H71-3+NC3H7O2H	3.20E+12	0	14900	REV/1.585E11 0.0E0 1.47E4/
711	C4H8-2+IC3H7O2=C4H71-3+IC3H7O2H	3.20E+12	0	14900	REV/1.585E11 0.0E0 1.47E4/
712	C4H8-2+PC4H9O2=C4H71-3+PC4H9O2H	3.20E+12	0	14900	REV/1.585E11 0.0E0 1.47E4/
713	C4H8-2+SC4H9O2=C4H71-3+SC4H9O2H	3.20E+12	0	14900	

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Table B .1. (cont.)

714	C4H8-1+HO2=>C4H8O1-2+OH	1.00E+12	0	14340	
715	C4H8-2+HO2=>C4H8O2-3+OH	5.62E+11	0	12310	
716	C4H8-2+CH3O2=>C4H8O2-3+CH3O	5.62E+11	0	12310	REV/4.75E12 0.0E0 -7.82E2/
717	PC4H8OH=C4H8-1+OH	1.08E+16	-0.699	28090	REV/4.75E12 0.0E0 -7.82E2/
718	SC4H8OH=C4H8-2+OH	3.38E+17	-1.253	29920	REV/2.0E12 0.0E0 0.0E0/
719	C4H8OH-1O2=PC4H8OH+O2	6.75E+20	-1.944	35520	REV/2.0E12 0.0E0 0.0E0/
720	C4H8OH-2O2=SC4H8OH+O2	7.69E+20	-1.968	35510	
721	C4H8OH-1O2=>C2H5CHO+CH2O+OH	1.00E+16	0	25000	
722	C4H8OH-2O2=>OH+2CH3CHO	1.00E+16	0	25000	REV/2.0E11 0.0E0 7.8E3/
723	C4H71-1=C2H2+C2H5	1.07E+15	-0.56	30320	REV/2.0E11 0.0E0 7.8E3/
724	C4H71-2=C3H4-A+CH3	9.59E+14	-0.71	31260	REV/2.0E11 0.0E0 7.8E3/
725	C4H71-4=C2H4+C2H3	8.77E+12	-0.22	36290	REV/1.0E11 0.0E0 7.8E3/
726	C4H72-2=C3H4-P+CH3	6.33E+10	0.52	30020	REV/4.0E13 0.0E0 1.3E3/
727	C4H71-3=C4H6+H	1.20E+14	0	49300	REV/1.149E13 6.0E-2 4.944E4/
728	C4H71-3+C2H5=C4H8-1+C2H4	2.59E+12	0	-131	REV/2.482E12 2.8E-1 6.633E4/
729	C4H71-3+CH3O=C4H8-1+CH2O	2.41E+13	0	0	REV/3.385E15 -7.8E-1 8.163E4/
730	C4H71-3+O=C2H3CHO+CH3	6.03E+13	0	0	REV/7.29E15 -1.09E0 1.553E4/
731	C4H71-3+HO2=C4H7O+OH	9.64E+12	0	0	REV/7.12E17 -1.67E0 2.029E4/
732	C4H71-3+CH3O2=C4H7O+CH3O	9.64E+12	0	0	REV/1.0E10 0.0E0 5.0E4/
733	C3H5-A+C4H71-3=C3H6+C4H6	6.31E+12	0	0	REV/1.0E11 0.0E0 1.7E4/
734	C4H71-3+O2=C4H6+HO2	1.00E+09	0	0	REV/1.066E13 0.0E0 5.681E4/
735	H+C4H71-3=C4H6+H2	3.16E+13	0	0	REV/3.211E12 0.0E0 4.984E4/
736	C2H5+C4H71-3=C4H6+C2H6	3.98E+12	0	0	REV/1.157E13 0.0E0 5.771E4/
737	C2H3+C4H71-3=C2H4+C4H6	3.98E+12	0	0	REV/2.0E10 0.0E0 0.0E0/
738	C4H71-3+C2H5O2=C4H7O+C2H5O	3.80E+12	0	-1200	REV/2.0E10 0.0E0 0.0E0/
739	IC3H7O2+C4H71-3=IC3H7O+C4H7O	3.80E+12	0	-1200	REV/2.0E10 0.0E0 0.0E0/
740	NC3H7O2+C4H71-3=NC3H7O+C4H7O	3.80E+12	0	-1200	REV/1.0E10 0.0E0 2.0E4/
741	C4H7O=CH3CHO+C2H3	7.94E+14	0	19000	REV/1.0E10 0.0E0 2.0E4/
742	C4H7O=C2H3CHO+CH3	7.94E+14	0	19000	REV/3.73E12 0.0E0 3.002E4/
743	C4H6+OH=C2H5+CH2CO	1.00E+12	0	0	REV/3.501E6 0.0E0 7.106E4/
744	C4H6+OH=CH2O+C3H5-A	1.00E+12	0	0	REV/5.437E11 0.0E0 1.855E4/
745	C4H6+OH=C2H3+CH3CHO	1.00E+12	0	0	REV/6.377E11 0.0E0 9.434E4/
746	C4H6+O=C2H4+CH2CO	1.00E+12	0	0	REV/1.075E12 0.0E0 7.905E4/
747	C4H6+O=CH2O+C3H4-A	1.00E+12	0	0	
748	C4H8O1-2+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
749	C4H8O1-2+H=>CH2O+C3H5-A+H2	5.00E+12	0	0	
750	C4H8O1-2+O=>CH2O+C3H5-A+OH	5.00E+12	0	0	
751	C4H8O1-2+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
752	C4H8O1-2+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
753	C4H8O1-2+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	
754	C4H8O1-3+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
755	C4H8O1-3+H=>CH2O+C3H5-A+H2	5.00E+12	0	0	
756	C4H8O1-3+O=>CH2O+C3H5-A+OH	5.00E+12	0	0	

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Table B .1. (cont.)

757	C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
758	C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
759	C4H8O1-3+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	
760	C4H8O1-4+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
761	C4H8O1-4+H=>CH2O+C3H5-A+H2	5.00E+12	0	0	
762	C4H8O1-4+O=>CH2O+C3H5-A+OH	5.00E+12	0	0	
763	C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
764	C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
765	C4H8O1-4+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	
766	C4H8O2-3+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
767	C4H8O2-3+H=>CH2O+C3H5-A+H2	5.00E+12	0	0	
768	C4H8O2-3+O=>CH2O+C3H5-A+OH	5.00E+12	0	0	
769	C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
770	C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
771	C4H8O2-3+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	REV/4.52E12 0.0E0 0.0E0/
772	PC4H9O2=PC4H9+O2	2.85E+20	-1.642	35930	REV/7.54E12 0.0E0 0.0E0/
773	SC4H9O2=SC4H9+O2	4.33E+22	-2.216	38160	REV/8.0E11 0.0E0 1.0E4/
774	SC4H9O2+CH2O=SC4H9O2H+HCO	5.60E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
775	SC4H9O2+CH3CHO=SC4H9O2H+CH3CO	2.80E+12	0	13600	REV/3.861E13 -7.96E-1 3.362E4/
776	SC4H9O2+HO2=SC4H9O2H+O2	1.75E+10	0	-3275	REV/2.281E13 7.5E-2 2.748E4/
777	IC3H7O2+PC4H9=IC3H7O+PC4H9O	7.00E+12	0	-1000	REV/3.942E15 -4.17E-1 2.919E4/
778	IC3H7O2+SC4H9=IC3H7O+SC4H9O	7.00E+12	0	-1000	REV/1.056E15 -6.11E-1 2.768E4/
779	NC3H7O2+PC4H9=NC3H7O+PC4H9O	7.00E+12	0	-1000	REV/1.825E17 -1.103E0 2.939E4/
780	NC3H7O2+SC4H9=NC3H7O+SC4H9O	7.00E+12	0	-1000	
781	2SC4H9O2=>O2+2SC4H9O	1.40E+16	-1.61	1860	
782	SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2	1.40E+16	-1.61	1860	
783	SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2	1.40E+16	-1.61	1860	
784	SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2	1.40E+16	-1.61	1860	
785	SC4H9O2+CH3O2=>SC4H9O+CH3O+O2	1.40E+16	-1.61	1860	
786	SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2	1.40E+16	-1.61	1860	
787	PC4H9O2+HO2=>PC4H9O+OH+O2	1.40E-14	-1.61	1860	
788	SC4H9O2+HO2=>SC4H9O+OH+O2	1.40E-14	-1.61	1860	REV/4.8E13 0.0E0 7.95E3/
789	H2+PC4H9O2=H+PC4H9O2H	3.01E+13	0	26030	REV/4.8E13 0.0E0 7.95E3/
790	H2+SC4H9O2=H+SC4H9O2H	3.01E+13	0	26030	REV/5.0E11 0.0E0 6.5E3/
791	C2H6+PC4H9O2=C2H5+PC4H9O2H	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
792	C2H6+SC4H9O2=C2H5+SC4H9O2H	1.70E+13	0	20460	REV/5.0E9 0.0E0 1.0E4/
793	PC4H9O2+C2H5CHO=PC4H9O2H+C2H5CO	2.00E+11	0	9500	REV/5.0E9 0.0E0 1.0E4/
794	SC4H9O2+C2H5CHO=SC4H9O2H+C2H5CO	2.00E+11	0	9500	REV/1.176E13 6.7E-2 2.611E4/
795	SC4H9O2+CH3=SC4H9O+CH3O	7.00E+12	0	-1000	REV/1.672E15 -5.34E-1 2.852E4/
796	SC4H9O2+C2H5=SC4H9O+C2H5O	7.00E+12	0	-1000	REV/2.852E15 -3.67E-1 2.919E4/
797	SC4H9O2+IC3H7=SC4H9O+IC3H7O	7.00E+12	0	-1000	REV/1.688E15 -5.03E-1 2.719E4/
798	SC4H9O2+NC3H7=SC4H9O+NC3H7O	7.00E+12	0	-1000	REV/2.342E15 -5.53E-1 2.687E4/
799	SC4H9O2+PC4H9=SC4H9O+PC4H9O	7.00E+12	0	-1000	REV/4.048E17 -1.045E0 2.858E4/
800	SC4H9O2+SC4H9=2SC4H9O	7.00E+12	0	-1000	REV/4.356E11 2.49E-1 1.353E4/

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Table B .1. (cont.)

801	SC4H9O2+C3H5-A=SC4H9O+C3H5O	7.00E+12	0	-1000	REV/8.0E11 0.0E0 1.0E4/
802	PC4H9O2+CH2O=PC4H9O2H+HCO	5.60E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
803	PC4H9O2+CH3CHO=PC4H9O2H+CH3CO	2.80E+12	0	13600	REV/4.357E13 -8.13E-1 3.363E4/
804	PC4H9O2+HO2=PC4H9O2H+O2	1.75E+10	0	-3275	REV/2.0E10 0.0E0 1.5E4/
805	C3H6+PC4H9O2=C3H5-A+PC4H9O2H	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
806	C3H6+SC4H9O2=C3H5-A+SC4H9O2H	3.24E+11	0	14900	REV/3.0E12 0.0E0 1.15E4/
807	C2H4+PC4H9O2=C2H3+PC4H9O2H	1.13E+13	0	30430	REV/3.0E12 0.0E0 1.15E4/
808	C2H4+SC4H9O2=C2H3+SC4H9O2H	1.13E+13	0	30430	REV/1.0E9 0.0E0 1.0E4/
809	CH3OH+PC4H9O2=CH2OH+PC4H9O2H	6.30E+12	0	19360	REV/1.0E9 0.0E0 1.0E4/
810	CH3OH+SC4H9O2=CH2OH+SC4H9O2H	6.30E+12	0	19360	REV/1.0E12 0.0E0 1.0E4/
811	C2H3CHO+PC4H9O2=C2H3CO+PC4H9O2H	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
812	C2H3CHO+SC4H9O2=C2H3CO+SC4H9O2H	2.80E+12	0	13600	REV/7.43E11 0.0E0 5.5E3/
813	CH4+PC4H9O2=CH3+PC4H9O2H	1.12E+13	0	24640	REV/7.43E11 0.0E0 5.5E3/
814	CH4+SC4H9O2=CH3+SC4H9O2H	1.12E+13	0	24640	REV/1.186E14 -7.63E-1 1.61E4/
815	C4H71-3+PC4H9O2=C4H7O+PC4H9O	7.00E+12	0	-1000	REV/2.251E14 -6.8E-1 1.558E4/
816	C4H71-3+SC4H9O2=C4H7O+SC4H9O	7.00E+12	0	-1000	REV/2.4E12 0.0E0 1.0E4/
817	H2O2+PC4H9O2=HO2+PC4H9O2H	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
818	H2O2+SC4H9O2=HO2+SC4H9O2H	2.40E+12	0	10000	
819	2PC4H9O2=>O2+2PC4H9O	1.40E+16	-1.61	1860	
820	PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2	1.40E+16	-1.61	1860	
821	PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2	1.40E+16	-1.61	1860	
822	PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2	1.40E+16	-1.61	1860	
823	PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2	1.40E+16	-1.61	1860	
824	PC4H9O2+CH3O2=>PC4H9O+CH3O+O2	1.40E+16	-1.61	1860	
825	PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2	1.40E+16	-1.61	1860	REV/6.199E12 -1.5E-2 2.663E4/
826	PC4H9O2+CH3=PC4H9O+CH3O	7.00E+12	0	-1000	REV/8.813E14 -6.17E-1 2.904E4/
827	PC4H9O2+C2H5=PC4H9O+C2H5O	7.00E+12	0	-1000	REV/1.503E15 -4.5E-1 2.971E4/
828	PC4H9O2+IC3H7=PC4H9O+IC3H7O	7.00E+12	0	-1000	REV/8.898E14 -5.86E-1 2.771E4/
829	PC4H9O2+NC3H7=PC4H9O+NC3H7O	7.00E+12	0	-1000	REV/1.235E15 -6.36E-1 2.739E4/
830	PC4H9O2+PC4H9=2PC4H9O	7.00E+12	0	-1000	REV/2.134E17 -1.128E0 2.91E4/
831	PC4H9O2+SC4H9=PC4H9O+SC4H9O	7.00E+12	0	-1000	REV/2.296E11 1.67E-1 1.405E4/
832	PC4H9O2+C3H5-A=PC4H9O+C3H5O	7.00E+12	0	-1000	REV/8.63E15 -7.43E-1 2.5E4/
833	PC4H9+HO2=PC4H9O+OH	7.00E+12	0	-1000	REV/1.491E18 -1.234E0 2.671E4/
834	SC4H9+HO2=SC4H9O+OH	7.00E+12	0	-1000	REV/5.398E14 -4.44E-1 2.924E4/
835	CH3O2+PC4H9=CH3O+PC4H9O	7.00E+12	0	-1000	REV/9.329E16 -9.36E-1 3.095E4/
836	CH3O2+SC4H9=CH3O+SC4H9O	7.00E+12	0	-1000	REV/1.178E8 1.712E0 -4.342E3/
837	PC4H9O2H=PC4H9O+OH	1.50E+16	0	42500	REV/1.589E8 1.778E0 -5.752E3/
838	SC4H9O2H=SC4H9O+OH	9.45E+15	0	41600	REV/5.0E10 0.0E0 3.457E3/
839	PC4H9O=NC3H7+CH2O	1.56E+21	-2.444	15230	REV/5.0E10 0.0E0 9.043E3/
840	SC4H9O=CH3+C2H5CHO	4.38E+16	-0.893	15200	REV/3.33E10 0.0E0 6.397E3/
841	SC4H9O=C2H5+CH3CHO	5.49E+22	-2.757	12650	REV/5.597E8 3.39E-1 1.197E4/

(cont. on next page)

Table B .1. (cont.)

842	PC4H9O2=C4H8OOH1-2	2.00E+11	0	26850	REV/3.231E9 -1.36E-1 7.871E3/
843	PC4H9O2=C4H8OOH1-3	2.50E+10	0	20850	REV/1.269E10 -5.23E-1 6.9E3/
844	PC4H9O2=C4H8OOH1-4	4.69E+09	0	22350	REV/7.442E11 -5.11E-1 1.394E4/
845	SC4H9O2=C4H8OOH2-1	3.00E+11	0	29400	REV/3.994E10 -1.96E-1 1.393E4/
846	SC4H9O2=C4H8OOH2-3	2.00E+11	0	26850	REV/9.302E10 -5.11E-1 8.944E3/
847	SC4H9O2=C4H8OOH2-4	3.75E+10	0	24400	REV/1.599E30 -6.283E0 2.035E4/
848	PC4H9O2=C4H8-1+HO2	5.04E+38	-8.11	40490	REV/2.595E33 -7.347E0 1.661E4/
849	SC4H9O2=C4H8-1+HO2	5.08E+42	-9.41	41490	REV/1.618E29 -5.793E0 1.83E4/
850	SC4H9O2=C4H8-2+HO2	5.04E+38	-8.11	40490	REV/1.0E11 0.0E0 1.1E4/
851	C4H8OOH1-2=C4H8-1+HO2	8.83E+16	-1.488	16260	REV/1.0E11 0.0E0 1.175E4/
852	C4H8OOH2-1=C4H8-1+HO2	4.85E+20	-2.574	21180	REV/1.0E11 0.0E0 1.175E4/
853	C4H8OOH2-3=C4H8-2+HO2	6.22E+19	-2.513	21020	
854	C4H8OOH1-2=>C4H8O1-2+OH	6.00E+11	0	22000	
855	C4H8OOH1-3=>C4H8O1-3+OH	7.50E+10	0	15250	
856	C4H8OOH1-4=>C4H8O1-4+OH	9.38E+09	0	6000	
857	C4H8OOH2-1=>C4H8O1-2+OH	6.00E+11	0	22000	
858	C4H8OOH2-3=>C4H8O2-3+OH	6.00E+11	0	22000	
859	C4H8OOH2-4=>C4H8O1-3+OH	7.50E+10	0	15250	REV/1.733E8 1.89E0 3.347E4/
860	C4H8OOH1-1=NC3H7CHO+OH	9.00E+14	0	1500	REV/1.99E10 1.34E0 3.551E4/
861	C4H8OOH2-2=C2H5COCH3+OH	9.00E+14	0	1500	
862	C4H8OOH1-3=>OH+CH2O+C3H6	6.64E+13	-0.16	29900	
863	C4H8OOH2-4=>OH+CH3CHO+C2H4	1.95E+18	-1.63	26790	REV/7.54E12 0.0E0 0.0E0/
864	C4H8OOH1-2O2=C4H8OOH1-2+O2	2.59E+24	-2.709	39860	REV/7.54E12 0.0E0 0.0E0/
865	C4H8OOH1-3O2=C4H8OOH1-3+O2	5.60E+22	-2.234	37960	REV/4.52E12 0.0E0 0.0E0/
866	C4H8OOH1-4O2=C4H8OOH1-4+O2	2.57E+20	-1.611	35680	REV/4.52E12 0.0E0 0.0E0/
867	C4H8OOH2-1O2=C4H8OOH2-1+O2	2.82E+20	-1.622	35700	REV/7.54E12 0.0E0 0.0E0/
868	C4H8OOH2-3O2=C4H8OOH2-3+O2	4.52E+22	-2.218	37880	REV/4.52E12 0.0E0 0.0E0/
869	C4H8OOH2-4O2=C4H8OOH2-4+O2	2.82E+20	-1.622	35700	REV/3.199E4 1.323E0 4.893E4/
870	C4H8OOH1-2O2=NC4KET12+OH	2.00E+11	0	26400	REV/1.435E3 1.486E0 4.474E4/
871	C4H8OOH1-3O2=NC4KET13+OH	2.50E+10	0	21400	REV/1.726E2 1.494E0 4.269E4/
872	C4H8OOH1-4O2=NC4KET14+OH	3.13E+09	0	19350	REV/3.626E2 1.835E0 5.005E4/
873	C4H8OOH2-1O2=NC4KET21+OH	1.00E+11	0	23850	REV/1.739E3 1.731E0 4.913E4/
874	C4H8OOH2-3O2=NC4KET23+OH	1.00E+11	0	23850	REV/1.021E2 1.843E0 4.392E4/
875	C4H8OOH2-4O2=NC4KET24+OH	1.25E+10	0	17850	
876	NC4KET12=>C2H5CHO+HCO+OH	1.05E+16	0	41600	
877	NC4KET13=>CH3CHO+CH2CHO+OH	1.05E+16	0	41600	
878	NC4KET14=>CH2CH2CHO+CH2O+OH	1.50E+16	0	42000	
879	NC4KET21=>CH2O+C2H5CO+OH	1.50E+16	0	42000	
880	NC4KET23=>CH3CHO+CH3CO+OH	1.05E+16	0	41600	
881	NC4KET24=>CH2O+CH3COCH2+OH	1.50E+16	0	42000	REV/1.527E9 9.6E-1 2.102E4/
882	C2H5COCH3+OH=CH2CH2COCH3+H2O	7.55E+09	0.97	1586	REV/1.586E13 -2.3E-1 2.862E4/

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Table B .1. (cont.)

883	C2H5COCH3+OH=CH3CHCOCH3+H2O	8.45E+11	0	-228	REV/6.628E13 -7.0E-1 2.767E4/
884	C2H5COCH3+OH=C2H5COCH2+H2O	5.10E+11	0	1192	REV/2.857E4 2.22E0 4.459E3/
885	C2H5COCH3+HO2=CH2CH2COCH3+H2O2	2.38E+04	2.55	16490	REV/2.229E13 -5.5E-1 6.08E3/
886	C2H5COCH3+HO2=CH3CHCOCH3+H2O2	2.00E+11	0	8698	REV/1.836E7 1.52E0 9.702E3/
887	C2H5COCH3+HO2=C2H5COCH2+H2O2	2.38E+04	2.55	14690	REV/4.616E11 -1.0E-2 9.882E3/
888	C2H5COCH3+O=CH2CH2COCH3+OH	2.25E+13	0	7700	REV/5.847E13 -2.3E-1 1.5E4/
889	C2H5COCH3+O=CH3CHCOCH3+OH	3.07E+13	0	3400	REV/6.592E13 -7.0E-1 1.519E4/
890	C2H5COCH3+O=C2H5COCH2+OH	5.00E+12	0	5962	REV/4.279E5 1.99E0 1.198E4/
891	C2H5COCH3+H=CH2CH2COCH3+H2	9.16E+06	2	7700	REV/1.934E7 1.77E0 1.689E4/
892	C2H5COCH3+H=CH3CHCOCH3+H2	4.46E+06	2	3200	REV/2.792E14 -7.0E-1 1.768E4/
893	C2H5COCH3+H=C2H5COCH2+H2	9.30E+12	0	6357	REV/1.74E10 3.2E-1 -1.895E3/
894	C2H5COCH3+O2=CH2CH2COCH3+HO2	2.05E+13	0	51310	REV/1.221E12 1.0E-1 -1.822E3/
895	C2H5COCH3+O2=CH3CHCOCH3+HO2	1.55E+13	0	41970	REV/1.118E13 -3.7E-1 2.988E3/
896	C2H5COCH3+O2=C2H5COCH2+HO2	2.05E+13	0	49150	REV/3.893E1 3.16E0 1.193E4/
897	C2H5COCH3+CH3=CH2CH2COCH3+CH4	3.19E+01	3.17	7172	REV/1.971E2 3.23E0 1.785E4/
898	C2H5COCH3+CH3=CH3CHCOCH3+CH4	1.74E+00	3.46	3680	REV/1.27E14 -7.0E-1 2.143E4/
899	C2H5COCH3+CH3=C2H5COCH2+CH4	1.62E+11	0	9630	REV/4.887E9 2.0E-2 9.007E3/
900	C2H5COCH3+CH3O=CH2CH2COCH3+CH3OH	2.17E+11	0	6460	REV/3.031E11 -2.0E-1 1.473E4/
901	C2H5COCH3+CH3O=CH3CHCOCH3+CH3OH	1.45E+11	0	2771	REV/3.14E12 -6.8E-1 1.425E4/
902	C2H5COCH3+CH3O=C2H5COCH2+CH3OH	2.17E+11	0	4660	REV/7.525E12 -5.1E-1 4.329E3/
903	C2H5COCH3+CH3O2=CH2CH2COCH3+CH3O2H	3.01E+12	0	19380	REV/4.641E14 -7.3E-1 9.612E3/
904	C2H5COCH3+CH3O2=CH3CHCOCH3+CH3O2H	2.00E+12	0	15250	REV/4.836E15 -1.2E0 9.572E3/
905	C2H5COCH3+CH3O2=C2H5COCH2+CH3O2H	3.01E+12	0	17580	REV/3.436E8 8.2E-1 1.403E4/
906	C2H5COCH3+C2H3=CH2CH2COCH3+C2H4	5.00E+11	0	10400	REV/1.914E10 6.0E-1 1.644E4/
907	C2H5COCH3+C2H3=CH3CHCOCH3+C2H4	3.00E+11	0	3400	REV/2.716E10 1.3E-1 1.495E4/
908	C2H5COCH3+C2H3=C2H5COCH2+C2H4	6.15E+10	0	4278	REV/9.549E12 -5.7E-1 1.399E4/
909	C2H5COCH3+C2H5=CH2CH2COCH3+C2H6	5.00E+10	0	13400	REV/5.319E14 -7.9E-1 1.86E4/
910	C2H5COCH3+C2H5=CH3CHCOCH3+C2H6	3.00E+10	0	8600	REV/6.136E15 -1.26E0 1.923E4/
911	C2H5COCH3+C2H5=C2H5COCH2+C2H6	5.00E+10	0	11600	REV/1.0E11 0.0E0 0.0E0/
912	CH3CHOOCOCH3=CH3CHCOCH3+O2	1.37E+17	-1.69	28460	REV/4.703E13 -5.2E-1 1.696E4/
913	CH3CHOOCOCH3=CH2CHOOHCOCH3	8.90E+12	0	29700	REV/7.0E10 0.0E0 7.8E3/
914	CH2CHOOHCOCH3=C2H3COCH3+HO2	2.03E+19	-2.35	14130	REV/1.5E11 0.0E0 8.3E3/
915	CH2CH2CHO=C2H4+HCO	3.13E+13	-0.52	24590	REV/1.0E11 0.0E0 0.0E0/
916	CH2CH2COCH3=C2H4+CH3CO	1.00E+14	0	18000	REV/1.0E11 0.0E0 0.0E0/
917	C2H5COCH2=CH2CO+C2H5	1.00E+14	0	35000	REV/5.0E12 0.0E0 1.2E3/
918	CH3CHCOCH3=C2H3COCH3+H	3.42E+16	-0.82	41770	REV/1.23E11 0.0E0 7.8E3/
919	CH3CHCOCH3=CH3CHCO+CH3	1.41E+15	-0.44	38340	REV/1.0E7 5.0E-1 4.0E3/
920	NC3H7CHO+O2=NC3H7CO+HO2	1.20E+05	2.5	37560	REV/1.553E4 2.32E0 2.805E4/

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Table B .1. (cont.)

921	NC3H7CHO+OH=NC3H7CO+H2O	2.00E+06	1.8	-1300	REV/3.03E6 1.746E0 1.678E4/
922	NC3H7CHO+H=NC3H7CO+H2	4.14E+09	1.12	2320	REV/2.258E9 6.07E-1 1.492E4/
923	NC3H7CHO+O=NC3H7CO+OH	5.94E+12	0	1868	REV/1.733E4 2.431E0 8.662E3/
924	NC3H7CHO+HO2=NC3H7CO+H2O2	4.09E+04	2.5	10200	REV/1.93E-3 4.8E0 1.921E4/
925	NC3H7CHO+CH3=NC3H7CO+CH4	2.89E-03	4.62	3210	REV/1.572E10 4.13E-1 1.799E4/
926	NC3H7CHO+CH3O=NC3H7CO+CH3OH	1.00E+12	0	3300	REV/3.371E5 1.986E0 7.067E3/
927	NC3H7CHO+CH3O2=NC3H7CO+CH3O2H	4.09E+04	2.5	10200	REV/1.23E7 1.494E0 1.882E4/
928	NC3H7CHO+OH=C3H6CHO-1+H2O	5.28E+09	0.97	1586	REV/9.102E3 2.444E0 1.974E4/
929	NC3H7CHO+OH=C3H6CHO-2+H2O	4.68E+07	1.61	-35	REV/1.428E2 3.4E0 2.551E4/
930	NC3H7CHO+OH=C3H6CHO-3+H2O	5.52E+02	3.12	-1176	REV/3.025E3 2.485E0 2.834E3/
931	NC3H7CHO+HO2=C3H6CHO-1+H2O2	2.38E+04	2.55	16490	REV/1.023E2 2.845E0 2.791E3/
932	NC3H7CHO+HO2=C3H6CHO-2+H2O2	9.64E+03	2.6	13910	REV/4.855E13 -2.59E-1 1.366E4/
933	NC3H7CHO+HO2=C3H6CHO-3+H2O2	3.44E+12	0.05	17880	REV/5.885E4 2.04E0 1.239E3/
934	NC3H7CHO+CH3O2=C3H6CHO-1+CH3O2H	2.38E+04	2.55	16490	REV/1.99E3 2.4E0 1.196E3/
935	NC3H7CHO+CH3O2=C3H6CHO-2+CH3O2H	9.64E+03	2.6	13910	REV/9.445E14 -7.04E-1 1.207E4/
936	NC3H7CHO+CH3O2=C3H6CHO-3+CH3O2H	3.44E+12	0.05	17880	REV/2.193E3 1.763E0 -1.1E3/
937	NC3H7CO=NC3H7+CO	1.00E+11	0	9600	REV/2.11E11 0.0E0 7.35E3/
938	C3H6CHO-1=C2H4+CH2CHO	7.40E+11	0	21970	REV/5.0E12 0.0E0 1.2E3/
939	C3H6CHO-3=C2H5CHCO+H	8.43E+15	-0.6	40400	REV/1.23E11 0.0E0 7.8E3/
940	C3H6CHO-3=C2H3CHO+CH3	3.17E+14	-0.39	29900	REV/5.0E12 0.0E0 2.9E3/
941	C3H6CHO-2=SC3H5CHO+H	4.95E+12	-0.15	31300	REV/1.0E11 0.0E0 6.0E3/
942	C3H6CHO-2=C3H6+HCO	8.25E+12	-0.18	21900	
943	C2H5CHCO+OH=>NC3H7+CO2	3.73E+12	0	-1010	
944	C2H5CHCO+H=>NC3H7+CO	4.40E+12	0	1459	
945	C2H5CHCO+O=>C3H6+CO2	3.20E+12	0	-437	REV/4.831E10 7.7E-1 3.709E4/
946	SC3H5CHO+OH=SC3H5CO+H2O	2.69E+10	0.76	-340	REV/1.0E11 0.0E0 6.0E3/
947	SC3H5CO=C3H5-S+CO	8.60E+15	0	23000	REV/1.066E13 -3.2E-1 1.789E4/
948	SC3H5CHO+HO2=SC3H5CO+H2O2	1.00E+12	0	11920	REV/4.313E13 1.0E-2 3.146E4/
949	SC3H5CHO+CH3=SC3H5CO+CH4	3.98E+12	0	8700	REV/1.308E12 1.0E-2 2.157E4/
950	SC3H5CHO+O=SC3H5CO+OH	7.18E+12	0	1389	REV/3.014E11 3.4E-1 2.394E3/
951	SC3H5CHO+O2=SC3H5CO+HO2	4.00E+13	0	37600	REV/1.079E12 1.0E-2 2.488E4/
952	SC3H5CHO+H=SC3H5CO+H2	2.60E+12	0	2600	
953	C2H3COCH3+OH=>CH3CHO+CH3CO	1.00E+11	0	0	
954	C2H3COCH3+OH=>CH2CO+C2H3+H2O	5.10E+11	0	1192	
955	C2H3COCH3+HO2=>CH2CHO+CH3CO+OH	6.03E+09	0	7949	
956	C2H3COCH3+HO2=>CH2CO+C2H3+H2O2	8.50E+12	0	20460	
957	C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O	3.97E+11	0	17050	
958	C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H	3.01E+12	0	17580	LOW/2.41E19 0.0E0 5.2576E4/ TROE/2.5E-1 7.5E2 1.0E-10 1.0E10/
959	IC4H10(+M)=CH3+IC3H7(+M)	4.83E+16	0	79900	REV/1.131E93 -2.2873E1 4.839E4/

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Table B .1. (cont.)

960	IC4H10=TC4H9+H	2.51E+98	-23.81	145300	REV/2.248E92 -2.2752E1 4.636E4/
961	IC4H10=IC4H9+H	9.85E+95	-23.11	147600	REV/1.084E0 3.613E0 9.213E3/
962	IC4H10+H=TC4H9+H2	6.02E+05	2.4	2583	REV/1.651E2 3.174E0 9.096E3/
963	IC4H10+H=IC4H9+H2	1.81E+06	2.54	6756	REV/1.485E-3 4.227E0 1.277E4/
964	IC4H10+CH3=TC4H9+CH4	9.04E-01	3.46	4598	REV/1.132E-1 3.838E0 1.103E4/
965	IC4H10+CH3=IC4H9+CH4	1.36E+00	3.65	7154	REV/5.584E-1 3.638E0 1.986E4/
966	IC4H10+OH=TC4H9+H2O	2.93E+04	2.531	-1659	REV/6.437E1 3.193E0 1.706E4/
967	IC4H10+OH=IC4H9+H2O	6.65E+04	2.665	-168.9	REV/3.2E11 0.0E0 1.23E4/
968	IC4H10+C2H5=IC4H9+C2H6	1.51E+12	0	10400	REV/3.0E11 0.0E0 2.1E4/
969	IC4H10+C2H5=TC4H9+C2H6	1.00E+11	0	7900	REV/3.231E0 3.529E0 3.5E3/
970	IC4H10+HO2=IC4H9+H2O2	6.12E+01	3.59	17160	REV/4.513E-1 3.528E0 2.723E3/
971	IC4H10+HO2=TC4H9+H2O2	4.33E+02	3.01	12090	REV/1.839E-1 3.596E0 6.368E3/
972	IC4H10+O=TC4H9+OH	1.97E+05	2.402	1150	REV/1.916E3 2.649E0 6.064E3/
973	IC4H10+O=IC4H9+OH	4.05E+07	2.034	5136	REV/9.402E8 4.21E-1 9.567E3/
974	IC4H10+CH3O=IC4H9+CH3OH	4.80E+11	0	7000	REV/7.344E5 1.0E0 9.657E3/
975	IC4H10+CH3O=TC4H9+CH3OH	1.90E+10	0	2800	REV/4.306E10 2.86E-1 -5.9E1/
976	IC4H10+O2=IC4H9+HO2	9.00E+13	0	52290	REV/9.442E7 8.65E-1 1.41E2/
977	IC4H10+O2=TC4H9+HO2	1.00E+13	0	48200	REV/2.135E0 3.464E0 3.026E3/
978	IC4H10+CH3O2=IC4H9+CH3O2H	2.08E+00	3.97	18280	REV/2.623E13 -5.06E-1 5.208E3/
979	IC4H10+C2H5O2=IC4H9+C2H5O2H	2.55E+13	0	20460	REV/2.147E12 -9.0E-3 9.57E3/
980	IC4H10+CH3CO3=IC4H9+CH3CO3H	2.55E+13	0	20460	REV/2.678E13 -5.09E-1 5.0E3/
981	IC4H10+NC3H7O2=IC4H9+NC3H7O2H	2.55E+13	0	20460	REV/2.688E13 -5.1E-1 5.0E3/
982	IC4H10+IC3H7O2=IC4H9+IC3H7O2H	2.55E+13	0	20460	REV/2.679E13 -5.09E-1 5.01E3/
983	IC4H10+IC4H9O2=IC4H9+IC4H9O2H	2.55E+13	0	20460	REV/2.684E13 -5.1E-1 5.01E3/
984	IC4H10+TC4H9O2=IC4H9+TC4H9O2H	2.55E+13	0	20460	REV/1.006E0 3.06E0 2.375E3/
985	IC4H10+O2CHO=IC4H9+HO2CHO	2.52E+13	0	20440	REV/1.893E1 2.72E0 4.678E3/
986	IC4H10+O2CHO=TC4H9+HO2CHO	2.80E+12	0	16010	REV/5.0E11 0.0E0 6.5E3/
987	IC4H10+SC4H9O2=IC4H9+SC4H9O2H	2.25E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
988	IC4H10+SC4H9O2=TC4H9+SC4H9O2H	2.80E+12	0	16000	REV/5.0E11 0.0E0 6.5E3/
989	IC4H10+PC4H9O2=IC4H9+PC4H9O2H	2.25E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
990	IC4H10+PC4H9O2=TC4H9+PC4H9O2H	2.80E+12	0	16000	REV/2.769E0 3.193E0 2.228E3/
991	IC4H10+CH3O2=TC4H9+CH3O2H	1.37E+02	3.12	13190	REV/1.0E11 0.0E0 1.0E4/
992	IC4H10+C2H5O2=TC4H9+C2H5O2H	2.80E+12	0	16000	REV/1.0E11 0.0E0 1.0E4/
993	IC4H10+CH3CO3=TC4H9+CH3CO3H	2.80E+12	0	16000	REV/1.0E11 0.0E0 1.0E4/
994	IC4H10+NC3H7O2=TC4H9+NC3H7O2H	2.80E+12	0	16000	REV/1.0E11 0.0E0 1.0E4/
995	IC4H10+IC3H7O2=TC4H9+IC3H7O2H	2.80E+12	0	16000	REV/1.0E11 0.0E0 1.0E4/
996	IC4H10+IC4H9O2=TC4H9+IC4H9O2H	2.80E+12	0	16000	REV/1.0E11 0.0E0 1.0E4/
997	IC4H10+TC4H9O2=TC4H9+TC4H9O2H	2.80E+12	0	16000	REV/2.25E11 0.0E0 1.23E4/
998	IC4H10+IC4H9=TC4H9+IC4H10	2.50E+10	0	7900	REV/3.712E15 -6.58E-1 2.654E4/

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Table B .1. (cont.)

999	IC4H9+HO2=IC4H9O+OH	7.00E+12	0	-1000	REV/4.083E18 -1.329E0 2.865E4/
1000	TC4H9+HO2=TC4H9O+OH	7.00E+12	0	-1000	REV/2.322E14 -3.59E-1 3.078E4/
1001	CH3O2+IC4H9=CH3O+IC4H9O	7.00E+12	0	-1000	REV/2.554E17 -1.03E0 3.289E4/
1002	CH3O2+TC4H9=CH3O+TC4H9O	7.00E+12	0	-1000	REV/6.25E11 5.1E-1 2.62E3/
1003	IC4H9=IC4H8+H	3.37E+13	0.124	33660	REV/1.89E3 2.67E0 6.85E3/
1004	IC4H9=C3H6+CH3	9.50E+11	0.773	30700	REV/1.06E12 5.1E-1 1.23E3/
1005	TC4H9=H+IC4H8	1.13E+12	0.703	36560	REV/1.648E0 3.325E0 2.55E4/
1006	TC4H9+O2=IC4H8+HO2	8.37E-01	3.59	11960	REV/4.158E-2 4.024E0 2.715E4/
1007	IC4H9+O2=IC4H8+HO2	1.07E+00	3.71	9322	REV/4.543E14 -5.26E-1 2.922E4/
1008	NC3H7O2+IC4H9=NC3H7O+IC4H9O	7.00E+12	0	-1000	REV/4.997E17 -1.197E0 3.133E4/
1009	NC3H7O2+TC4H9=NC3H7O+TC4H9O	7.00E+12	0	-1000	REV/4.183E11 1.82E-1 1.35E4/
1010	NC3H7O2+IC4H7=NC3H7O+IC4H7O	7.00E+12	0	-1000	REV/1.007E15 -4.68E-1 2.841E4/
1011	SC4H9O2+IC4H9=SC4H9O+IC4H9O	7.00E+12	0	-1000	REV/1.108E18 -1.139E0 3.052E4/
1012	SC4H9O2+TC4H9=SC4H9O+TC4H9O	7.00E+12	0	-1000	REV/5.31E14 -5.51E-1 2.893E4/
1013	PC4H9O2+IC4H9=PC4H9O+IC4H9O	7.00E+12	0	-1000	REV/5.841E17 -1.222E0 3.104E4/
1014	PC4H9O2+TC4H9=PC4H9O+TC4H9O	7.00E+12	0	-1000	REV/4.89E11 1.57E-1 1.321E4/
1015	PC4H9O2+IC4H7=PC4H9O+IC4H7O	7.00E+12	0	-1000	REV/9.277E11 2.4E-1 1.269E4/
1016	SC4H9O2+IC4H7=SC4H9O+IC4H7O	7.00E+12	0	-1000	REV/2.26E12 0.0E0 0.0E0/
1017	IC4H9O2=IC4H9+O2	6.64E+19	-1.575	36080	REV/1.41E13 0.0E0 0.0E0/
1018	TC4H9O2=TC4H9+O2	3.33E+24	-2.472	37870	REV/5.0E11 0.0E0 6.5E3/
1019	IC4H9O2+C4H10=IC4H9O2H+SC4H9	1.12E+13	0	17700	REV/5.0E11 0.0E0 6.5E3/
1020	TC4H9O2+C4H10=TC4H9O2H+SC4H9	1.12E+13	0	17700	REV/5.0E11 0.0E0 6.5E3/
1021	IC4H9O2+C4H10=IC4H9O2H+PC4H9	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
1022	TC4H9O2+C4H10=TC4H9O2H+PC4H9	1.70E+13	0	20460	REV/9.811E12 1.6E-1 2.902E4/
1023	IC3H7O2+IC4H9=IC3H7O+IC4H9O	7.00E+12	0	-1000	REV/1.079E16 -5.11E-1 3.113E4/
1024	IC3H7O2+TC4H9=IC3H7O+TC4H9O	7.00E+12	0	-1000	REV/9.035E9 8.68E-1 1.33E4/
1025	IC3H7O2+IC4H7=IC3H7O+IC4H7O	7.00E+12	0	-1000	REV/2.0E10 0.0E0 1.5E4/
1026	IC4H9O2+C3H6=IC4H9O2H+C3H5-A	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
1027	TC4H9O2+C3H6=TC4H9O2H+C3H5-A	3.24E+11	0	14900	REV/3.16E11 0.0E0 1.3E4/
1028	IC4H9O2+IC4H8=IC4H9O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1029	TC4H9O2+IC4H8=TC4H9O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1030	PC4H9O2+IC4H8=PC4H9O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1031	SC4H9O2+IC4H8=SC4H9O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1032	IC3H7O2+IC4H8=IC3H7O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1033	NC3H7O2+IC4H8=NC3H7O2H+IC4H7	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1034	IC4H9O2+C4H8-1=IC4H9O2H+C4H71-3	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1035	TC4H9O2+C4H8-1=TC4H9O2H+C4H71-3	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1036	IC4H9O2+C4H8-2=IC4H9O2H+C4H71-3	1.40E+12	0	14900	REV/3.16E11 0.0E0 1.3E4/
1037	TC4H9O2+C4H8-2=TC4H9O2H+C4H71-3	1.40E+12	0	14900	
1038	CC4H8O+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
1039	CC4H8O+H=>CH2O+C3H5-A+H2	3.51E+07	2	5000	

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Table B .1. (cont.)

1040	CC4H8O+O=>CH2O+C3H5-A+OH	1.12E+14	0	5200	
1041	CC4H8O+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
1042	CC4H8O+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
1043	CC4H8O+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	REV/1.0E11 0.0E0 1.0E4/
1044	C2H4+TC4H9O2=C2H3+TC4H9O2H	7.00E+11	0	17110	REV/7.5E8 0.0E0 1.28E3/
1045	TC4H9O2+CH4=TC4H9O2H+CH3	1.13E+13	0	20460	REV/4.8E13 0.0E0 7.95E3/
1046	H2+TC4H9O2=H+TC4H9O2H	3.01E+13	0	26030	REV/5.0E11 0.0E0 6.5E3/
1047	TC4H9O2+C2H6=TC4H9O2H+C2H5	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
1048	TC4H9O2+C3H8=TC4H9O2H+IC3H7	2.00E+12	0	17000	REV/5.0E11 0.0E0 6.5E3/
1049	TC4H9O2+C3H8=TC4H9O2H+NC3H7	1.70E+13	0	20460	REV/1.0E9 0.0E0 1.0E4/
1050	TC4H9O2+CH3OH=TC4H9O2H+CH2OH	6.30E+12	0	19360	REV/3.061E12 0.0E0 2.21E4/
1051	TC4H9O2+C2H5OH=TC4H9O2H+PC2H4OH	6.30E+12	0	19360	REV/2.04E12 0.0E0 1.774E4/
1052	TC4H9O2+C2H5OH=TC4H9O2H+SC2H4OH	4.20E+12	0	15000	REV/1.0E12 0.0E0 1.0E4/
1053	IC4H9O2+CH3CHO=IC4H9O2H+CH3CO	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
1054	TC4H9O2+CH3CHO=TC4H9O2H+CH3CO	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
1055	IC4H9O2+C2H3CHO=IC4H9O2H+C2H3CO	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
1056	TC4H9O2+C2H3CHO=TC4H9O2H+C2H3CO	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
1057	IC4H9O2+C2H5CHO=IC4H9O2H+C2H5CO	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
1058	TC4H9O2+C2H5CHO=TC4H9O2H+C2H5CO	2.80E+12	0	13600	REV/3.843E13 -7.95E-1 3.362E4/
1059	IC4H9O2+HO2=IC4H9O2H+O2	1.75E+10	0	-3275	REV/3.85E13 -7.95E-1 3.362E4/
1060	TC4H9O2+HO2=TC4H9O2H+O2	1.75E+10	0	-3275	REV/2.4E12 0.0E0 1.0E4/
1061	IC4H9O2+H2O2=IC4H9O2H+HO2	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
1062	TC4H9O2+H2O2=TC4H9O2H+HO2	2.40E+12	0	10000	REV/2.5E10 0.0E0 1.01E4/
1063	IC4H9O2+CH2O=IC4H9O2H+HCO	1.30E+11	0	9000	REV/2.5E10 0.0E0 1.01E4/
1064	TC4H9O2+CH2O=TC4H9O2H+HCO	1.30E+11	0	9000	
1065	IC4H9O2+CH3O2=>IC4H9O+CH3O+O2	1.40E+16	-1.61	1860	
1066	TC4H9O2+CH3O2=>TC4H9O+CH3O+O2	1.40E+16	-1.61	1860	
1067	IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2	1.40E+16	-1.61	1860	
1068	TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2	1.40E+16	-1.61	1860	
1069	IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2	1.40E+16	-1.61	1860	
1070	TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2	1.40E+16	-1.61	1860	
1071	2IC4H9O2=>O2+2IC4H9O	1.40E+16	-1.61	1860	
1072	IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2	1.40E+16	-1.61	1860	
1073	2TC4H9O2=>O2+2TC4H9O	1.40E+16	-1.61	1860	
1074	IC4H9O2+PC4H9O2=>IC4H9O+PC4H9O+O2	1.40E+16	-1.61	1860	
1075	TC4H9O2+PC4H9O2=>TC4H9O+PC4H9O+O2	1.40E+16	-1.61	1860	
1076	IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2	1.40E+16	-1.61	1860	
1077	TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2	1.40E+16	-1.61	1860	
1078	IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2	1.40E+16	-1.61	1860	
1079	TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2	1.40E+16	-1.61	1860	
1080	IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2	1.40E+16	-1.61	1860	
1081	TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2	1.40E+16	-1.61	1860	
1082	IC4H9O2+HO2=>IC4H9O+OH+O2	1.40E+16	-1.61	1860	
1083	TC4H9O2+HO2=>TC4H9O+OH+O2	1.40E+16	-1.61	1860	REV/5.72E12 3.0E-3 2.802E4/
1084	IC4H9O2+CH3=IC4H9O+CH3O	7.00E+12	0	-1000	REV/8.133E14 -5.99E-1 3.043E4/

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Table B .1. (cont.)

1085	IC4H9O2+C2H5=IC4H9O+C2H5O	7.00E+12	0	-1000	REV/1.387E15 -4.32E-1 3.11E4/
1086	IC4H9O2+IC3H7=IC4H9O+IC3H7O	7.00E+12	0	-1000	REV/8.212E14 -5.68E-1 2.91E4/
1087	IC4H9O2+NC3H7=IC4H9O+NC3H7O	7.00E+12	0	-1000	REV/1.139E15 -6.18E-1 2.878E4/
1088	IC4H9O2+PC4H9=IC4H9O+PC4H9O	7.00E+12	0	-1000	REV/1.969E17 -1.11E0 3.049E4/
1089	IC4H9O2+SC4H9=IC4H9O+SC4H9O	7.00E+12	0	-1000	REV/4.9E14 -5.33E-1 3.032E4/
1090	IC4H9O2+IC4H9=2IC4H9O	7.00E+12	0	-1000	REV/5.39E17 -1.204E0 3.243E4/
1091	IC4H9O2+TC4H9=IC4H9O+TC4H9O	7.00E+12	0	-1000	REV/2.119E11 1.84E-1 1.544E4/
1092	IC4H9O2+C3H5-A=IC4H9O+C3H5O	7.00E+12	0	-1000	REV/1.095E14 -7.45E-1 1.749E4/
1093	IC4H9O2+C4H71-3=IC4H9O+C4H7O	7.00E+12	0	-1000	REV/4.512E11 1.75E-1 1.46E4/
1094	IC4H9O2+IC4H7=IC4H9O+IC4H7O	7.00E+12	0	-1000	REV/7.824E11 2.29E-1 2.834E4/
1095	TC4H9O2+CH3=TC4H9O+CH3O	7.00E+12	0	-1000	REV/1.112E14 -3.72E-1 3.075E4/
1096	TC4H9O2+C2H5=TC4H9O+C2H5O	7.00E+12	0	-1000	REV/1.898E14 -2.06E-1 3.142E4/
1097	TC4H9O2+IC3H7=TC4H9O+IC3H7O	7.00E+12	0	-1000	REV/1.123E14 -3.41E-1 2.942E4/
1098	TC4H9O2+NC3H7=TC4H9O+NC3H7O	7.00E+12	0	-1000	REV/1.558E14 -3.92E-1 2.91E4/
1099	TC4H9O2+PC4H9=TC4H9O+PC4H9O	7.00E+12	0	-1000	REV/2.693E16 -8.83E-1 3.081E4/
1100	TC4H9O2+SC4H9=TC4H9O+SC4H9O	7.00E+12	0	-1000	REV/6.703E13 -3.07E-1 3.064E4/
1101	TC4H9O2+IC4H9=TC4H9O+IC4H9O	7.00E+12	0	-1000	REV/7.373E16 -9.78E-1 3.275E4/
1102	TC4H9O2+TC4H9=2TC4H9O	7.00E+12	0	-1000	REV/2.898E10 4.11E-1 1.576E4/
1103	TC4H9O2+C3H5-A=TC4H9O+C3H5O	7.00E+12	0	-1000	REV/1.497E13 -5.19E-1 1.781E4/
1104	TC4H9O2+C4H71-3=TC4H9O+C4H7O	7.00E+12	0	-1000	REV/6.172E10 4.01E-1 1.492E4/
1105	TC4H9O2+IC4H7=TC4H9O+IC4H7O	7.00E+12	0	-1000	REV/2.0E10 0.0E0 8.0E3/
1106	IC4H9O2+C2H4=IC4H9O2H+C2H3	2.00E+11	0	6000	REV/7.5E8 0.0E0 1.28E3/
1107	IC4H9O2+CH4=IC4H9O2H+CH3	1.13E+13	0	20460	REV/4.8E13 0.0E0 7.95E3/
1108	H2+IC4H9O2=H+IC4H9O2H	3.01E+13	0	26030	REV/5.0E11 0.0E0 6.5E3/
1109	IC4H9O2+C2H6=IC4H9O2H+C2H5	1.70E+13	0	20460	REV/5.0E11 0.0E0 6.5E3/
1110	IC4H9O2+C3H8=IC4H9O2H+IC3H7	2.00E+12	0	17000	REV/5.0E11 0.0E0 6.5E3/
1111	IC4H9O2+C3H8=IC4H9O2H+NC3H7	1.70E+13	0	20460	REV/1.0E9 0.0E0 1.0E4/
1112	IC4H9O2+CH3OH=IC4H9O2H+CH2OH	6.30E+12	0	19360	REV/3.061E12 0.0E0 2.21E4/
1113	IC4H9O2+C2H5OH=IC4H9O2H+PC2H4OH	6.30E+12	0	19360	REV/2.04E12 0.0E0 1.774E4/
1114	IC4H9O2+C2H5OH=IC4H9O2H+SC2H4OH	4.20E+12	0	15000	REV/1.233E8 1.712E0 -2.942E3/
1115	IC4H9O2H=IC4H9O+OH	1.50E+16	0	42500	REV/6.677E6 1.939E0 -2.582E3/
1116	TC4H9O2H=TC4H9O+OH	5.95E+15	0	42540	REV/1.38E13 -2.5E-1 7.213E4/
1117	IC4H9O+HO2=IC3H7CHO+H2O2	1.00E+12	0	0	REV/4.209E13 8.0E-2 1.036E5/
1118	IC4H9O+OH=IC3H7CHO+H2O	1.81E+13	0	0	REV/3.368E14 8.0E-2 8.892E4/
1119	IC4H9O+CH3=IC3H7CHO+CH4	2.40E+13	0	0	REV/1.415E12 8.0E-2 8.635E4/
1120	IC4H9O+O=IC3H7CHO+OH	6.00E+12	0	0	REV/1.069E13 8.0E-2 8.844E4/
1121	IC4H9O+H=IC3H7CHO+H2	1.99E+13	0	0	REV/1.139E10 1.08E0 2.5E3/

(cont. on next page)

Table B .1. (cont.)

1122	IC4H9O=IC3H7CHO+H	4.00E+14	0	21500	REV/1.877E2 2.796E0 4.591E3/
1123	IC4H9O=CH2O+IC3H7	2.00E+14	0	17500	REV/1.5E11 0.0E0 1.19E4/
1124	TC4H9O=CH3COCH3+CH3	9.56E+22	-2.548	18650	REV/7.026E8 5.64E-1 3.32E4/
1125	IC4H9O+O2=IC3H7CHO+HO2	1.93E+11	0	1660	REV/1.0E11 0.0E0 3.2E4/
1126	TC4H9O+O2=IC4H8O+HO2	8.10E+11	0	4700	REV/1.392E10 5.5E-1 7.205E4/
1127	IC4H8O=IC3H7CHO	4.18E+13	0	52720	REV/9.609E5 1.069E0 3.656E4/
1128	IC4H8O+OH=IC3H6CHO+H2O	1.25E+12	0	0	REV/9.063E4 1.175E0 2.167E4/
1129	IC4H8O+H=IC3H6CHO+H2	1.25E+12	0	0	REV/1.049E8 4.8E-1 2.066E4/
1130	IC4H8O+HO2=IC3H6CHO+H2O2	2.50E+12	0	15000	REV/2.04E9 3.6E-2 2.307E4/
1131	IC4H8O+CH3O2=IC3H6CHO+CH3O2H	2.50E+12	0	19000	REV/3.307E6 7.29E-1 3.321E4/
1132	IC4H8O+CH3=IC3H6CHO+CH4	5.00E+10	0	10000	REV/4.704E4 1.156E0 2.025E4/
1133	IC4H8O+O=IC3H6CHO+OH	1.25E+12	0	0	REV/2.0E14 0.0E0 0.0E0/
1134	IC3H7CHO=TC3H6CHO+H	2.30E+18	-0.91	92000	REV/1.81E13 0.0E0 0.0E0/
1135	IC3H7CHO=IC3H7+HCO	1.13E+17	-0.03	79760	REV/7.987E11 -6.2E-2 1.036E4/
1136	IC3H7CHO+HO2=IC3H7CO+H2O2	3.00E+12	0	11920	REV/3.366E12 -4.2E-1 1.105E4/
1137	IC3H7CHO+HO2=TC3H6CHO+H2O2	8.00E+10	0	11920	REV/2.325E13 -6.0E-2 2.563E4/
1138	IC3H7CHO+CH3=IC3H7CO+CH4	3.98E+12	0	8700	REV/7.052E11 -6.0E-2 1.574E4/
1139	IC3H7CHO+O=IC3H7CO+OH	7.18E+12	0	1389	REV/1.625E11 2.7E-1 -3.432E3/
1140	IC3H7CHO+O2=IC3H7CO+HO2	4.00E+13	0	37600	REV/1.164E10 7.5E-1 3.12E4/
1141	IC3H7CHO+OH=IC3H7CO+H2O	2.69E+10	0.76	-340	REV/1.194E13 -9.0E-2 2.981E4/
1142	IC3H7CHO+OH=TC3H6CHO+H2O	1.68E+12	0	-781	REV/1.196E9 6.33E-1 1.704E4/
1143	IC3H7CHO+H=IC3H7CO+H2	2.60E+12	0	2600	REV/6.388E5 1.99E0 1.913E4/
1144	IC3H7CHO+OH=IC3H6CHO+H2O	3.12E+06	2	-298	REV/3.33E4 2.21E0 3.468E3/
1145	IC3H7CHO+HO2=IC3H6CHO+H2O2	2.74E+04	2.55	15500	REV/2.377E5 2.04E0 3.742E3/
1146	IC3H7CHO+CH3O2=IC3H6CHO+CH3O2H	4.76E+04	2.55	16490	REV/1.5E11 0.0E0 4.81E3/
1147	IC3H7CO=IC3H7+CO	2.87E+20	-2.194	14970	REV/1.0E11 0.0E0 7.8E3/
1148	IC3H6CHO=C3H6+HCO	1.03E+15	-0.62	23170	REV/1.0E11 0.0E0 7.8E3/
1149	IC3H6CHO=C2H3CHO+CH3	2.43E+13	-0.27	22470	REV/9.93E11 0.0E0 -9.6E2/
1150	IC4H8OH=IC4H8+OH	9.23E+14	-0.562	28050	REV/1.2E11 0.0E0 -1.1E3/
1151	IO2C4H8OH=IC4H8OH+O2	1.92E+21	-2.347	35790	
1152	IO2C4H8OH=>CH3COCH3+CH2O+OH	1.25E+10	0	18900	REV/1.815E11 -5.07E-1 8.946E3/
1153	IC4H9O2=IC4H8O2H-I	7.50E+10	0	24400	REV/2.027E9 1.23E-1 1.694E4/
1154	TC4H9O2=TC4H8O2H-I	9.00E+11	0	34500	REV/5.085E6 7.8E-1 1.588E4/
1155	IC4H9O2=IC4H8O2H-T	1.00E+11	0	29200	REV/2.996E26 -5.331E0 2.124E4/
1156	IC4H9O2=IC4H8+HO2	2.27E+35	-7.22	39490	REV/6.344E31 -7.203E0 1.716E4/
1157	TC4H9O2=IC4H8+HO2	7.61E+42	-9.41	41490	REV/2.26E12 0.0E0 0.0E0/
1158	IC4H8OOH-IO2=IC4H8O2H-I+O2	1.44E+20	-1.627	35690	REV/2.26E12 0.0E0 0.0E0/
1159	TC4H8OOH-IO2=TC4H8O2H-I+O2	5.17E+22	-2.257	37800	REV/1.41E13 0.0E0 0.0E0/
1160	IC4H8OOH-TO2=IC4H8O2H-T+O2	2.27E+27	-3.233	39640	REV/1.986E3 1.455E0 4.442E4/

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Table B .1. (cont.)

1161	IC4H8OOH-IO2=IC4KETII+OH	5.00E+10	0	21400	REV/1.91E5 1.24E0 5.383E4/
1162	IC4H8OOH-TO2=IC4KETIT+OH	4.00E+11	0	31500	REV/6.36E8 9.1E-2 1.172E4/
1163	TC4H8OOH-IO2=TIC4H7Q2-I	7.50E+10	0	24400	REV/1.0E11 0.0E0 1.06E4/
1164	TIC4H7Q2-I=IC4H7OOH+HO2	1.94E+20	-2.19	22590	REV/8.986E8 -8.8E-2 1.19E4/
1165	IC4H8OOH-IO2=IIC4H7Q2-I	3.75E+10	0	24400	REV/9.448E7 4.06E-1 2.12E4/
1166	IC4H8OOH-IO2=IIC4H7Q2-T	1.00E+11	0	29200	REV/5.088E9 9.1E-2 2.182E4/
1167	IC4H8OOH-TO2=TIC4H7Q2-I	6.00E+11	0	34500	REV/8.5E10 0.0E0 1.06E4/
1168	IIC4H7Q2-I=AC3H5OOH+CH2O2H	7.63E+19	-1.74	38310	REV/1.0E11 0.0E0 7.8E3/
1169	IIC4H7Q2-T=IC4H7OOH+HO2	4.08E+17	-1.56	18390	REV/1.869E11 1.1E0 3.684E4/
1170	CH2O2H=CH2O+OH	9.00E+14	0	1500	
1171	IC4KETII=>CH2O+C2H5CO+OH	1.50E+16	0	42000	
1172	IC4KETIT=>CH3COCH3+HCO+OH	9.50E+15	0	42540	REV/3.97E11 0.0E0 1.262E4/
1173	TC4H8O2H-I=IC4H8+HO2	1.07E+20	-2.085	19390	REV/3.97E11 0.0E0 1.262E4/
1174	IC4H8O2H-T=IC4H8+HO2	1.53E+16	-1.109	17560	
1175	IC4H8O2H-I=>CC4H8O+OH	2.00E+11	0	19500	
1176	IC4H8O2H-T=>IC4H8O+OH	1.38E+12	0	14800	
1177	TC4H8O2H-I=>IC4H8O+OH	4.00E+12	0	17000	
1178	IC4H8O2H-I=>OH+CH2O+C3H6	8.45E+15	-0.68	29170	REV/1.561E56 -1.2293E1 2.61E4/
1179	IC4H8=C3H5-T+CH3	1.92E+66	-14.22	128100	REV/1.428E55 -1.1738E1 2.64E4/
1180	IC4H8=IC4H7+H	3.07E+55	-11.49	114300	REV/6.093E26 -4.209E0 2.72E4/
1181	IC4H8+H=C3H6+CH3	5.68E+33	-5.72	20000	REV/6.32E4 2.528E0 1.816E4/
1182	IC4H8+H=IC4H7+H2	3.40E+05	2.5	2492	
1183	IC4H8+O=>CH2CO+2CH3	3.33E+07	1.76	76	
1184	IC4H8+O=>IC3H6CO+2H	1.66E+07	1.76	76	REV/1.164E10 7.09E-1 2.189E4/
1185	IC4H8+O=IC4H7+OH	1.21E+11	0.7	7633	REV/7.495E2 3.082E0 2.289E4/
1186	IC4H8+CH3=IC4H7+CH4	4.42E+00	3.5	5675	REV/2.073E6 1.933E0 1.358E4/
1187	IC4H8+HO2=IC4H7+H2O2	1.93E+04	2.6	13910	REV/6.514E-7 4.9E0 -3.468E3/
1188	IC4H8+O2CHO=IC4H7+HO2CHO	1.93E+04	2.6	13910	REV/5.848E12 -3.2E-1 8.83E2/
1189	IC4H8+O2=IC4H7+HO2	6.00E+12	0	39900	REV/4.4E20 -1.33E0 6.061E4/
1190	IC4H8+C3H5-A=IC4H7+C3H6	7.94E+11	0	20500	REV/5.592E20 -1.27E0 8.217E4/
1191	IC4H8+C3H5-S=IC4H7+C3H6	7.94E+11	0	20500	REV/5.592E20 -1.27E0 8.017E4/
1192	IC4H8+C3H5-T=IC4H7+C3H6	7.94E+11	0	20500	REV/1.025E7 1.922E0 3.027E4/
1193	IC4H8+OH=IC4H7+H2O	5.20E+06	2	-298	REV/4.538E0 3.06E0 2.169E4/
1194	IC4H8+O=IC3H7+HCO	1.58E+07	1.76	-1216	REV/4.034E7 1.488E0 1.199E4/
1195	IC4H8+CH3O2=IC4H7+CH3O2H	1.93E+04	2.6	13910	REV/1.0E12 0.0E0 7.5E3/
1196	IC4H8+HO2=IC4H8O+OH	1.29E+12	0	13340	REV/3.372E13 -5.77E-1 7.301E4/
1197	IC4H7+O2=IC3H5CHO+OH	2.47E+13	-0.45	23020	REV/1.7E12 -4.07E-1 8.825E4/
1198	IC4H7+O2=CH3COCH2+CH2O	7.14E+15	-1.21	21050	
1199	IC4H7+O2=>C3H4-A+CH2O+OH	7.29E+29	-5.71	21450	REV/2.844E16 -5.19E-1 6.673E4/

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Table B .1. (cont.)

1200	IC4H7+O=IC3H5CHO+H	6.03E+13	0	0	REV/1.649E38 -7.768E0 2.254E4/
1201	IC4H7=C3H4-A+CH3	1.23E+47	-9.74	74260	REV/2.138E11 3.49E-1 1.506E4/
1202	CH3O2+IC4H7=CH3O+IC4H7O	7.00E+12	0	-1000	REV/3.418E12 5.0E-2 1.082E4/
1203	IC4H7+HO2=IC4H7O+OH	7.00E+12	0	-1000	REV/1.0E11 0.0E0 1.26E4/
1204	IC4H7O=C3H5-T+CH2O	2.93E+21	-2.391	35590	REV/4.233E11 -1.64E-1 3.167E4/
1205	IC4H7O=IC4H6OH	1.39E+11	0	15600	REV/6.67E13 -1.05E-1 1.841E4/
1206	IC4H7O=IC3H5CHO+H	5.00E+13	0	29100	REV/5.614E2 2.98E0 1.399E3/
1207	IC4H6OH+H2=IC4H7OH+H	2.16E+04	2.38	18990	REV/6.0E13 0.0E0 3.99E4/
1208	IC4H6OH+HO2=IC4H7OH+O2	5.57E+13	-0.315	862	REV/2.101E7 2.153E0 1.773E4/
1209	IC4H6OH+CH2O=IC4H7OH+HCO	6.30E+08	1.9	18190	REV/2.814E-1 3.9E0 6.521E3/
1210	IC4H6OH+IC4H8=IC4H7OH+IC4H7	4.70E+02	3.3	19840	REV/1.0E14 0.0E0 0.0E0/
1211	IC4H7OH=IC4H6OH+H	4.90E+16	-0.4	89850	REV/7.83E5 2.05E0 1.358E4/
1212	IC4H7OH+HO2=IC4H6OH+H2O2	7.64E+03	2.712	13930	REV/1.0E11 0.0E0 9.2E3/
1213	IC4H6OH=C3H4-A+CH2OH	7.24E+19	-1.859	57050	REV/6.312E10 -1.4E-1 3.898E4/
1214	IC4H7O+O2=IC3H5CHO+HO2	3.00E+10	0	1649	REV/8.93E14 -8.0E-1 7.85E4/
1215	IC4H7O+HO2=IC3H5CHO+H2O2	3.00E+11	0	0	REV/7.261E16 -4.7E-1 9.529E4/
1216	IC4H7O+CH3=IC3H5CHO+CH4	2.40E+13	0	0	REV/3.052E14 -4.7E-1 9.272E4/
1217	IC4H7O+O=IC3H5CHO+OH	6.00E+12	0	0	REV/9.076E15 -4.7E-1 1.1E5/
1218	IC4H7O+OH=IC3H5CHO+H2O	1.81E+13	0	0	REV/2.305E15 -4.7E-1 9.481E4/
1219	IC4H7O+H=IC3H5CHO+H2	1.99E+13	0	0	REV/4.4E10 7.8E-1 3.608E4/
1220	IC3H5CHO+OH=IC3H5CO+H2O	2.69E+10	0.76	-340	REV/9.709E12 -3.1E-1 1.688E4/
1221	IC3H5CHO+HO2=IC3H5CO+H2O2	1.00E+12	0	11920	REV/3.928E13 2.0E-2 3.045E4/
1222	IC3H5CHO+CH3=IC3H5CO+CH4	3.98E+12	0	8700	REV/1.191E12 2.0E-2 2.056E4/
1223	IC3H5CHO+O=IC3H5CO+OH	7.18E+12	0	1389	REV/1.824E11 3.11E-1 5.337E3/
1224	IC3H5CHO+O2=IC3H5CO+HO2	2.00E+13	0	40700	REV/9.822E11 2.0E-2 2.387E4/
1225	IC3H5CHO+H=IC3H5CO+H2	2.60E+12	0	2600	REV/1.51E11 0.0E0 4.809E3/
1226	IC3H5CO=C3H5-T+CO	1.28E+20	-1.89	34460	REV/2.018E17 -1.2E0 2.101E4/
1227	TC3H6CHO+HO2=TC3H6OCHO+OH	9.64E+12	0	0	REV/2.173E8 8.0E-1 1.424E4/
1228	TC3H6OCHO=CH3COCH3+HCO	3.98E+13	0	9700	REV/1.3E13 0.0E0 1.2E3/
1229	TC3H6CHO=IC3H5CHO+H	1.33E+14	0.01	39340	REV/1.3E13 0.0E0 4.8E3/
1230	TC3H6CHO=IC3H6CO+H	4.09E+14	-0.072	42410	REV/1.319E5 2.47E0 3.55E3/
1231	TC3H6CHO+H2=IC3H7CHO+H	2.16E+05	2.38	18990	REV/1.0E11 0.0E0 0.0E0/
1232	IC4H7OOH=IC4H7O+OH	6.40E+15	0	45550	REV/4.0E13 0.0E0 0.0E0/
1233	IC4H7OH=IC4H7O+H	5.97E+16	-0.56	105900	REV/1.0E13 0.0E0 1.2E3/
1234	IC4H8OH=IC4H7OH+H	1.71E+12	0.277	38850	REV/7.16E5 2.44E0 1.631E4/
1235	IC4H7O+H2=IC4H7OH+H	9.05E+06	2	17830	REV/3.0E13 0.0E0 0.0E0/
1236	IC4H7OH=IC4H7+OH	7.31E+16	-0.41	79700	REV/3.02E11 0.0E0 1.816E4/
1237	IC4H7O+CH2O=IC4H7OH+HCO	1.15E+11	0	1280	REV/1.229E7 1.99E0 1.742E4/

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Table B .1. (cont.)

1238	TC3H6CHO+CH2O=IC3H7CHO+HCO	2.52E+08	1.9	18190	REV/6.613E0 3.39E0 8.672E3/
1239	TC3H6CHO+IC4H8=IC3H7CHO+IC4H7	4.70E+02	3.3	19840	REV/2.577E14 -4.3E-1 5.548E4/
1240	IC3H6CO+OH=IC3H7+CO2	1.73E+12	0	-1010	REV/5.0E13 0.0E0 0.0E0/
1241	TC3H6OHCHO=TC3H6CHO+OH	9.99E+20	-1.46	87480	REV/1.81E13 0.0E0 0.0E0/
1242	TC3H6OHCHO=TC3H6OH+HCO	5.16E+23	-1.9	76850	REV/1.0E12 0.0E0 0.0E0/
1243	TC3H6OH=CH3COCH3+H	5.00E+13	0	21860	REV/1.3E13 0.0E0 1.56E3/
1244	TC3H6OH=IC3H5OH+H	6.20E+15	-0.66	40340	REV/5.0E13 0.0E0 0.0E0/
1245	IC3H5OH=C3H5-T+OH	7.37E+19	-0.94	109100	REV/1.99E17 -2.1E0 0.0E0/
1246	TC3H6O2CHO=TC3H6CHO+O2	2.46E+25	-4.065	27080	REV/3.014E12 -5.16E-1 1.711E4/
1247	TC3H6O2CHO=IC3H5O2HCHO	6.00E+11	0	29880	REV/1.628E12 -5.16E-1 2.51E4/
1248	TC3H6O2CHO=TC3H6O2HCO	1.00E+11	0	25750	REV/2.23E11 0.0E0 1.06E4/
1249	IC3H5O2HCHO=IC3H5CHO+HO2	8.94E+20	-2.44	15030	
1250	TC3H6O2HCO=>CH3COCH3+CO+OH	4.24E+18	-1.43	4800	REV/6.529E17 -1.19E0 2.561E4/
1251	TC3H6OH+O2=CH3COCH3+HO2	2.23E+13	0	0	REV/1.009E9 9.0E-1 3.154E4/
1252	IC3H6CO+OH=TC3H6OH+CO	2.00E+12	0	-1010	REV/1.39E11 -2.0E-1 1.731E4/
1253	TC3H6CHO+O2=IC3H5CHO+HO2	2.73E-19	0	7240	
1254	TC3H6CHO+O2=>CH3COCH3+CO+OH	3.62E-20	0	0	REV/1.236E14 -2.4E-1 4.335E4/
1255	TC3H6CHO+HO2=IC3H7CHO+O2	3.68E+12	0	1310	REV/2.207E15 -8.5E-1 6.79E4/
1256	TC3H6CHO+CH3=IC3H5CHO+CH4	3.01E+12	-0.32	-131	REV/2.23E11 0.0E0 1.06E4/
1257	TC4H8CHO=IC3H5CHO+CH3	1.00E+13	0	26290	REV/1.0E11 0.0E0 6.0E3/
1258	TC4H8CHO=IC4H8+HCO	8.52E+12	0	20090	REV/2.0E12 0.0E0 0.0E0/
1259	O2C4H8CHO=TC4H8CHO+O2	1.52E+19	-1.44	34510	REV/1.173E13 -6.8E-1 1.488E4/
1260	O2C4H8CHO=O2HC4H8CO	2.16E+11	0	15360	REV/1.5E11 0.0E0 4.809E3/
1261	O2HC4H8CO=IC4H8O2H-T+CO	3.30E+22	-2.72	11760	REV/1.0E10 0.0E0 9.0E3/
1262	IC4H7O+IC4H8=IC4H7OH+IC4H7	2.70E+11	0	4000	
1263	IC4H6OH+HO2=>CH2CCH2OH+CH2O+OH	1.45E+13	0	0	REV/2.75E11 -5.0E-2 2.847E4/
1264	IC4H8+CH2CCH2OH=IC4H7+C3H5OH	7.94E+11	0	20500	REV/3.01E9 0.0E0 2.583E3/
1265	C3H5OH+HO2=CH2CCH2OH+H2O2	1.76E+09	0.28	22590	REV/1.457E12 5.0E-2 1.741E4/
1266	C3H5OH+OH=CH2CCH2OH+H2O	5.06E+12	0	5960	REV/2.594E4 2.55E0 2.121E3/
1267	C3H5OH+H=CH2CCH2OH+H2	3.90E+05	2.5	5821	REV/4.833E10 3.8E-1 -4.92E2/
1268	C3H5OH+O2=CH2CCH2OH+HO2	4.00E+13	0	60690	REV/4.17E11 5.0E-2 4.81E3/
1269	C3H5OH+CH3=CH2CCH2OH+CH4	2.40E+11	0	8030	REV/3.0E13 0.0E0 0.0E0/
1270	IC4H7OH=CH2CCH2OH+CH3	1.25E+20	-0.98	98570	REV/1.0E14 0.0E0 0.0E0/
1271	C3H5OH=CH2CCH2OH+H	2.84E+19	-1.05	111100	
1272	CH2CCH2OH+O2=>CH2OH+CO+CH2O	4.34E+12	0	0	REV/1.61E40 -8.58E0 2.033E4/
1273	CH2CCH2OH=C2H2+CH2OH	2.16E+40	-8.31	45110	REV/8.5E12 0.0E0 2.0E3/
1274	CH2CCH2OH=C3H4-A+OH	6.70E+16	-1.11	42580	REV/3.61E13 0.0E0 0.0E0/
1275	NC5H12=C5H11-1+H	1.38E+17	-0.36	101200	REV/3.61E13 0.0E0 0.0E0/
1276	NC5H12=C5H11-2+H	3.33E+18	-0.763	98800	REV/3.61E13 0.0E0 0.0E0/
1277	NC5H12=C5H11-3+H	1.60E+18	-0.758	98790	REV/4.0E12 0.0E0 -5.96E2/
1278	NC5H12=CH3+PC4H9	6.10E+22	-1.862	89430	REV/4.0E12 0.0E0 -5.96E2/
1279	NC5H12=NC3H7+C2H5	3.08E+24	-2.269	88440	REV/1.972E1 3.386E0 8.61E3/

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Table B .1. (cont.)

1280	NC5H12+H=C5H11-1+H2	1.88E+05	2.75	6280	REV/1.128E1 3.439E0 9.236E3/
1281	NC5H12+H=C5H11-2+H2	2.60E+06	2.4	4471	REV/1.171E1 3.434E0 9.244E3/
1282	NC5H12+H=C5H11-3+H2	1.30E+06	2.4	4471	REV/1.172E7 1.5E0 1.881E4/
1283	NC5H12+OH=C5H11-1+H2O	1.05E+10	0.97	1590	REV/4.297E3 2.543E0 1.962E4/
1284	NC5H12+OH=C5H11-2+H2O	9.34E+07	1.61	-35	REV/4.459E3 2.538E0 1.963E4/
1285	NC5H12+OH=C5H11-3+H2O	4.67E+07	1.61	-35	REV/1.139E2 3.041E0 5.684E3/
1286	NC5H12+O=C5H11-1+OH	2.09E+06	2.424	4766	REV/2.678E0 3.459E0 6.199E3/
1287	NC5H12+O=C5H11-2+OH	1.19E+06	2.439	2846	REV/2.779E0 3.454E0 6.207E3/
1288	NC5H12+O=C5H11-3+OH	5.95E+05	2.439	2846	REV/8.653E-2 3.84E0 1.102E4/
1289	NC5H12+CH3=C5H11-1+CH4	9.04E-01	3.65	7154	REV/6.65E2 2.726E0 1.388E4/
1290	NC5H12+CH3=C5H11-2+CH4	1.68E+05	2.133	7574	REV/6.901E2 2.721E0 1.389E4/
1291	NC5H12+CH3=C5H11-3+CH4	8.40E+04	2.133	7574	REV/2.477E0 3.531E0 3.49E3/
1292	NC5H12+HO2=C5H11-1+H2O2	4.08E+01	3.59	17160	REV/3.173E-1 3.714E0 2.483E3/
1293	NC5H12+HO2=C5H11-2+H2O2	1.26E+02	3.37	13720	REV/3.293E-1 3.709E0 2.491E3/
1294	NC5H12+HO2=C5H11-3+H2O2	6.32E+01	3.37	13720	REV/4.818E1 3.086E0 1.895E3/
1295	NC5H12+CH3O2=C5H11-1+CH3O2H	4.08E+01	3.59	17160	REV/6.173E0 3.269E0 8.88E2/
1296	NC5H12+CH3O2=C5H11-2+CH3O2H	1.26E+02	3.37	13720	REV/6.406E0 3.264E0 8.96E2/
1297	NC5H12+CH3O2=C5H11-3+CH3O2H	6.32E+01	3.37	13720	REV/3.2E11 0.0E0 1.23E4/
1298	NC5H12+C2H5=C5H11-1+C2H6	1.00E+11	0	13400	REV/1.0E11 0.0E0 1.29E4/
1299	NC5H12+C2H5=C5H11-2+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
1300	NC5H12+C2H5=C5H11-3+C2H6	5.00E+10	0	10400	REV/2.6E12 0.0E0 2.54E4/
1301	NC5H12+C2H3=C5H11-1+C2H4	1.00E+12	0	18000	REV/2.0E12 0.0E0 2.42E4/
1302	NC5H12+C2H3=C5H11-2+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
1303	NC5H12+C2H3=C5H11-3+C2H4	4.00E+11	0	16800	REV/1.0E11 0.0E0 1.29E4/
1304	NC5H12+C5H11-1=C5H11-2+NC5H12	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
1305	NC5H12+C5H11-1=C5H11-3+NC5H12	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.23E4/
1306	NC5H12+C5H11-2=C5H11-3+NC5H12	5.00E+10	0	12300	REV/1.368E0 3.11E0 2.295E3/
1307	NC5H12+O2CHO=C5H11-1+HO2CHO	1.68E+13	0	20440	REV/4.306E3 2.13E0 4.147E3/
1308	NC5H12+O2CHO=C5H11-2+HO2CHO	1.12E+13	0	17690	REV/4.318E3 2.13E0 4.149E3/
1309	NC5H12+O2CHO=C5H11-3+HO2CHO	5.60E+12	0	17690	REV/1.2E10 0.0E0 9.2E3/
1310	NC5H12+CH3O=C5H11-1+CH3OH	3.00E+11	0	7000	REV/9.0E9 0.0E0 7.2E3/
1311	NC5H12+CH3O=C5H11-2+CH3OH	2.20E+11	0	5000	REV/9.0E9 0.0E0 7.2E3/
1312	NC5H12+CH3O=C5H11-3+CH3OH	1.10E+11	0	5000	REV/2.311E10 2.88E-1 4.46E2/
1313	NC5H12+O2=C5H11-1+HO2	4.20E+13	0	52800	REV/6.37E8 6.91E-1 2.31E2/
1314	NC5H12+O2=C5H11-2+HO2	2.80E+13	0	50160	REV/6.611E8 6.86E-1 2.39E2/
1315	NC5H12+O2=C5H11-3+HO2	1.40E+13	0	50160	REV/8.8E3 2.48E0 6.13E3/
1316	C5H11-1=C2H4+NC3H7	3.21E+12	0.451	29430	REV/2.5E11 5.1E-1 2.62E3/
1317	C5H11-1=H+C5H10-1	3.35E+11	0.608	35640	REV/1.602E8 7.56E-1 2.22E4/
1318	C5H11-1=C5H11-2	3.88E+09	0.353	19760	REV/8.8E3 2.48E0 6.13E3/

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Table B .1. (cont.)

1319	C5H11-2=C3H6+C2H5	1.22E+12	0.635	29360	REV/4.24E11 5.1E-1 1.23E3/
1320	C5H11-2=C5H10-1+H	2.35E+10	1.011	36680	REV/2.5E11 5.1E-1 2.62E3/
1321	C5H11-2=C5H10-2+H	3.99E+11	0.41	35220	REV/1.76E4 2.48E0 6.13E3/
1322	C5H11-3=C4H8-1+CH3	6.34E+10	1.119	30460	REV/2.5E11 5.1E-1 2.62E3/
1323	C5H11-3=C5H10-2+H	8.28E+11	0.405	35230	REV/4.0E12 0.0E0 -5.96E2/
1324	C5H10-1=C2H5+C3H5-A	9.86E+21	-2.086	75060	REV/3.096E5 2.53E0 2.032E4/
1325	C5H10-1+H=C5H91-3+H2	3.38E+05	2.36	207	REV/2.777E2 3.17E0 1.124E4/
1326	C5H10-1+H=C5H91-4+H2	1.30E+06	2.4	4471	REV/2.193E3 2.96E0 1.102E4/
1327	C5H10-1+H=C5H91-5+H2	6.65E+05	2.54	6756	REV/2.658E5 2.6E0 1.923E4/
1328	C5H10-1+O=C5H91-3+OH	6.60E+05	2.43	1210	REV/5.169E1 3.22E0 7.505E3/
1329	C5H10-1+O=C5H91-4+OH	5.51E+05	2.45	2830	REV/1.419E3 2.85E0 6.915E3/
1330	C5H10-1+O=C5H91-5+OH	9.80E+05	2.43	4750	REV/1.097E5 2.81E0 3.335E4/
1331	C5H10-1+OH=C5H91-3+H2O	2.76E+04	2.64	-1919	REV/4.319E4 2.38E0 2.189E4/
1332	C5H10-1+OH=C5H91-4+H2O	4.67E+07	1.61	-35	REV/7.524E7 1.39E0 2.1E4/
1333	C5H10-1+OH=C5H91-5+H2O	5.27E+09	0.97	1586	REV/8.84E1 3.48E0 2.459E4/
1334	C5H10-1+CH3=C5H91-3+CH4	3.69E+00	3.31	4002	REV/8.426E-3 4.23E0 1.273E4/
1335	C5H10-1+CH3=C5H91-4+CH4	1.51E+00	3.46	5481	REV/3.895E-2 4.07E0 1.189E4/
1336	C5H10-1+CH3=C5H91-5+CH4	4.52E-01	3.65	7154	REV/3.665E10 4.9E-1 -1.52E2/
1337	C5H10-1+O2=C5H91-3+HO2	2.20E+12	0	37220	REV/7.76E7 1.09E0 -1.072E3/
1338	C5H10-1+O2=C5H91-4+HO2	2.00E+13	0	49640	REV/1.797E9 7.5E-1 -9.32E2/
1339	C5H10-1+O2=C5H91-5+HO2	3.00E+13	0	52290	REV/1.136E5 2.39E0 1.433E4/
1340	C5H10-1+HO2=C5H91-3+H2O2	4.82E+03	2.55	10530	REV/5.292E1 3.04E0 4.372E3/
1341	C5H10-1+HO2=C5H91-4+H2O2	9.64E+03	2.6	13910	REV/2.017E3 2.64E0 4.446E3/
1342	C5H10-1+HO2=C5H91-5+H2O2	2.38E+04	2.55	16490	REV/2.366E5 2.21E0 1.131E4/
1343	C5H10-1+CH3O2=C5H91-3+CH3O2H	4.82E+03	2.55	10530	REV/1.102E2 2.86E0 1.352E3/
1344	C5H10-1+CH3O2=C5H91-4+CH3O2H	9.64E+03	2.6	13910	REV/4.2E3 2.47E0 1.426E3/
1345	C5H10-1+CH3O2=C5H91-5+CH3O2H	2.38E+04	2.55	16490	REV/1.769E1 3.09E0 2.699E4/
1346	C5H10-1+CH3O=C5H91-3+CH3OH	4.00E+01	2.9	8609	REV/1.493E7 7.9E-1 9.611E3/
1347	C5H10-1+CH3O=C5H91-4+CH3OH	1.45E+11	0	4571	REV/3.45E8 4.5E-1 8.988E3/
1348	C5H10-1+CH3O=C5H91-5+CH3OH	2.17E+11	0	6458	REV/4.561E6 2.06E0 1.975E4/
1349	C5H10-2+H=C5H91-3+H2	1.73E+05	2.5	2492	REV/4.361E6 2.1E0 2.033E4/
1350	C5H10-2+H=C5H92-4+H2	3.38E+05	2.36	207	REV/3.085E4 2.54E0 1.103E4/
1351	C5H10-2+H=C5H92-5+H2	6.65E+05	2.54	6756	REV/5.107E6 1.98E0 1.831E4/
1352	C5H10-2+O=C5H91-3+OH	4.41E+05	2.42	3150	REV/5.617E6 2.17E0 1.924E4/
1353	C5H10-2+O=C5H92-4+OH	9.90E+05	2.43	1210	REV/1.996E4 2.42E0 6.931E3/
1354	C5H10-2+O=C5H92-5+OH	9.80E+05	2.43	4750	REV/3.562E8 1.56E0 3.211E4/
1355	C5H10-2+OH=C5H91-3+H2O	3.12E+06	2	-298	REV/1.546E6 2.38E0 3.336E4/

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Table B .1. (cont.)

1356	C5H10-2+OH=C5H92-4+H2O	2.76E+04	2.64	-1919	REV/1.058E9 9.6E-1 2.102E4/
1357	C5H10-2+OH=C5H92-5+H2O	5.27E+09	0.97	1586	REV/1.522E3 3.06E0 2.341E4/
1358	C5H10-2+CH3=C5H91-3+CH4	2.21E+00	3.5	5675	REV/1.245E3 3.05E0 2.461E4/
1359	C5H10-2+CH3=C5H92-4+CH4	3.69E+00	3.31	4002	REV/5.478E-1 3.64E0 1.191E4/
1360	C5H10-2+CH3=C5H92-5+CH4	4.52E-01	3.65	7154	REV/1.581E12 -1.1E-1 - 3.26E2/
1361	C5H10-2+O2=C5H91-3+HO2	3.30E+12	0	39900	REV/5.163E11 7.0E-2 - 1.36E2/
1362	C5H10-2+O2=C5H92-4+HO2	2.20E+12	0	37220	REV/2.528E10 3.2E-1 - 9.16E2/
1363	C5H10-2+O2=C5H92-5+HO2	3.00E+13	0	52290	REV/6.532E6 1.84E0 1.486E4/
1364	C5H10-2+HO2=C5H91-3+H2O2	9.64E+03	2.6	13910	REV/1.6E6 1.96E0 1.435E4/
1365	C5H10-2+HO2=C5H92-4+H2O2	4.82E+03	2.55	10530	REV/2.837E4 2.22E0 4.462E3/
1366	C5H10-2+HO2=C5H92-5+H2O2	2.38E+04	2.55	16490	REV/1.36E7 1.66E0 1.184E4/
1367	C5H10-2+CH3O2=C5H91-3+CH3O2H	9.64E+03	2.6	13910	REV/3.332E6 1.79E0 1.133E4/
1368	C5H10-2+CH3O2=C5H92-4+CH3O2H	4.82E+03	2.55	10530	REV/5.908E4 2.04E0 1.442E3/
1369	C5H10-2+CH3O2=C5H92-5+CH3O2H	2.38E+04	2.55	16490	REV/1.144E3 2.54E0 2.751E4/
1370	C5H10-2+CH3O=C5H91-3+CH3OH	9.00E+01	2.95	11990	REV/2.491E2 2.67E0 2.701E4/
1371	C5H10-2+CH3O=C5H92-4+CH3OH	4.00E+01	2.9	8609	REV/4.853E9 2.0E-2 9.004E3/
1372	C5H10-2+CH3O=C5H92-5+CH3OH	2.17E+11	0	6458	REV/6.088E15 -1.07E0 1.572E4/
1373	C5H91-3+HO2=C5H9O1-3+OH	9.64E+12	0	0	REV/5.946E17 -1.65E0 2.048E4/
1374	C5H91-3+CH3O2=C5H9O1-3+CH3O	9.64E+12	0	0	REV/3.893E14 -7.2E-1 1.833E4/
1375	C5H91-3+C2H5O2=C5H9O1-3+C2H5O	9.64E+12	0	0	REV/7.027E15 -1.24E0 1.589E4/
1376	C5H92-4+HO2=C5H9O2-4+OH	9.64E+12	0	0	REV/6.863E17 -1.82E0 2.065E4/
1377	C5H92-4+CH3O2=C5H9O2-4+CH3O	9.64E+12	0	0	REV/4.493E14 -8.9E-1 1.849E4/
1378	C5H92-4+C2H5O2=C5H9O2-4+C2H5O	9.64E+12	0	0	REV/1.0E11 0.0E0 7.8E3/
1379	C5H91-3=C4H6+CH3	7.55E+14	-0.52	38520	REV/2.5E11 5.1E-1 2.62E3/
1380	C5H91-3=C5H81-3+H	4.73E+11	0.636	42640	REV/1.0E11 0.0E0 7.8E3/
1381	C5H91-4=C3H6+C2H3	5.81E+11	0.17	35850	REV/1.0E11 0.0E0 7.8E3/
1382	C5H91-5=C2H4+C3H5-A	7.16E+16	-1.42	17750	REV/1.0E13 0.0E0 1.2E3/
1383	C5H92-4=C5H81-3+H	2.02E+15	-0.34	46030	REV/2.0E11 0.0E0 7.8E3/
1384	C5H92-5=C2H4+C3H5-S	8.90E+16	-1.18	42180	REV/1.0E11 0.0E0 9.6E3/
1385	C5H9O1-3=C2H3CHO+C2H5	3.13E+19	-1.85	10670	REV/1.0E11 0.0E0 9.6E3/
1386	C5H9O1-3=C2H5CHO+C2H3	1.42E+18	-1.56	23340	REV/1.0E11 0.0E0 1.5E4/
1387	C5H81-3+OH=CH2O+C4H71-3	1.00E+12	0	0	REV/1.0E11 0.0E0 1.5E4/
1388	C5H81-3+OH=C2H3CHO+C2H5	1.00E+12	0	0	REV/1.0E11 0.0E0 1.5E4/
1389	C5H81-3+OH=CH3CHO+C3H5-S	1.00E+12	0	0	REV/1.0E11 0.0E0 9.6E3/
1390	C5H9O2-4=SC3H5CHO+CH3	5.98E+15	-1.13	9941	REV/1.0E11 0.0E0 9.6E3/
1391	C5H9O2-4=CH3CHO+C3H5-S	1.07E+22	-2.66	29650	REV/8.0E12 0.0E0 -5.96E2/
1392	C5H10-2=CH3+C4H71-3	6.49E+19	-1.367	76320	REV/1.307E0 3.42E0 2.781E4/
1393	C5H11-1+O2=C5H10-1+HO2	8.37E-01	3.59	11960	REV/2.021E1 3.137E0 2.274E4/
1394	C5H11-2+O2=C5H10-1+HO2	5.35E-01	3.71	9322	REV/1.406E0 3.738E0 2.559E4/

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Table B .1. (cont.)

1395	C5H11-2+O2=C5H10-2+HO2	1.07E+00	3.71	9322	REV/1.355E0 3.743E0 2.558E4/
1396	C5H11-3+O2=C5H10-2+HO2	2.14E+00	3.71	9322	REV/1.944E15 -4.79E-1 2.621E4/
1397	C5H11-1+HO2=C5H11O-1+OH	9.00E+12	0	-1000	REV/3.143E17 -1.132E0 2.822E4/
1398	C5H11-2+HO2=C5H11O-2+OH	9.00E+12	0	-1000	REV/3.019E17 -1.127E0 2.821E4/
1399	C5H11-3+HO2=C5H11O-3+OH	9.00E+12	0	-1000	REV/1.216E14 -1.8E-1 3.045E4/
1400	C5H11-1+CH3O2=C5H11O-1+CH3O	9.00E+12	0	-1000	REV/1.966E16 -8.33E-1 3.246E4/
1401	C5H11-2+CH3O2=C5H11O-2+CH3O	9.00E+12	0	-1000	REV/1.889E16 -8.28E-1 3.245E4/
1402	C5H11-3+CH3O2=C5H11O-3+CH3O	9.00E+12	0	-1000	REV/1.44E10 0.0E0 1.5E4/
1403	C5H11O2-1+NC5H12=C5H11O2H-1+C5H11-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1404	C5H11O2-2+NC5H12=C5H11O2H-2+C5H11-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1405	C5H11O2-3+NC5H12=C5H11O2H-3+C5H11-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1406	C5H11O2-1+NC5H12=C5H11O2H-1+C5H11-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1407	C5H11O2-2+NC5H12=C5H11O2H-2+C5H11-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1408	C5H11O2-3+NC5H12=C5H11O2H-3+C5H11-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1409	C5H11O2-1+NC5H12=C5H11O2H-1+C5H11-3	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1410	C5H11O2-2+NC5H12=C5H11O2H-2+C5H11-3	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1411	C5H11O2-3+NC5H12=C5H11O2H-3+C5H11-3	4.03E+12	0	17700	REV/5.94E13 -1.3E-1 2.991E4/
1412	C5H11-1+C5H11O2-1=2C5H11O-1	9.00E+12	0	-1000	REV/5.285E13 -1.16E-1 2.96E4/
1413	C5H11-1+C5H11O2-2=C5H11O-1+C5H11O-2	9.00E+12	0	-1000	REV/1.053E14 -1.16E-1 2.96E4/
1414	C5H11-1+C5H11O2-3=C5H11O-1+C5H11O-3	9.00E+12	0	-1000	REV/9.604E15 -7.83E-1 3.192E4/
1415	C5H11-2+C5H11O2-1=C5H11O-2+C5H11O-1	9.00E+12	0	-1000	REV/8.544E15 -7.69E-1 3.162E4/
1416	C5H11-2+C5H11O2-2=2C5H11O-2	9.00E+12	0	-1000	REV/1.703E16 -7.69E-1 3.162E4/
1417	C5H11-2+C5H11O2-3=C5H11O-2+C5H11O-3	9.00E+12	0	-1000	REV/9.225E15 -7.78E-1 3.192E4/
1418	C5H11-3+C5H11O2-1=C5H11O-3+C5H11O-1	9.00E+12	0	-1000	REV/8.206E15 -7.64E-1 3.161E4/
1419	C5H11-3+C5H11O2-2=C5H11O-3+C5H11O-2	9.00E+12	0	-1000	REV/1.636E16 -7.64E-1 3.161E4/
1420	C5H11-3+C5H11O2-3=2C5H11O-3	9.00E+12	0	-1000	
1421	C5H11O2-1+C5H11O2-2=>O2+C5H11O-1+C5H11O-2	1.40E+16	-1.61	1860	
1422	C5H11O2-1+C5H11O2-3=>O2+C5H11O-1+C5H11O-3	1.40E+16	-1.61	1860	
1423	C5H11O2-1+CH3O2=>O2+C5H11O-1+CH3O	1.40E+16	-1.61	1860	
1424	2C5H11O2-1=>O2+2C5H11O-1	1.40E+16	-1.61	1860	REV/2.4E12 0.0E0 1.0E4/
1425	H2O2+C5H11O2-1=HO2+C5H11O2H-1	2.40E+12	0	10000	REV/3.746E13 -7.91E-1 3.362E4/
1426	C5H11O2-1+HO2=C5H11O2H-1+O2	1.75E+10	0	-3275	
1427	C5H11O2-2+CH3O2=>O2+C5H11O-2+CH3O	1.40E+16	-1.61	1860	
1428	C5H11O2-2+C5H11O2-3=>C5H11O-2+C5H11O-3+O2	1.40E+16	-1.61	1860	
1429	2C5H11O2-2=>O2+2C5H11O-2	1.40E+16	-1.61	1860	REV/2.4E12 0.0E0 1.0E4/
1430	H2O2+C5H11O2-2=HO2+C5H11O2H-2	2.40E+12	0	10000	REV/4.38E13 -8.12E-1 3.364E4/
1431	C5H11O2-2+HO2=C5H11O2H-2+O2	1.75E+10	0	-3275	
1432	C5H11O2-3+CH3O2=>O2+C5H11O-3+CH3O	1.40E+16	-1.61	1860	
1433	2C5H11O2-3=>O2+2C5H11O-3	1.40E+16	-1.61	1860	REV/2.4E12 0.0E0 1.0E4/
1434	H2O2+C5H11O2-3=HO2+C5H11O2H-3	2.40E+12	0	10000	REV/4.38E13 -8.12E-1 3.364E4/
1435	C5H11O2-3+HO2=C5H11O2H-3+O2	1.75E+10	0	-3275	REV/2.927E7 1.932E0 -3.022E3/

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Table B .1. (cont.)

1436	C5H11O2H-1=C5H11O-1+OH	1.50E+16	0	42500	REV/1.403E7 1.968E0 - 4.252E3/
1437	C5H11O2H-2=C5H11O-2+OH	9.45E+15	0	41600	REV/2.797E7 1.968E0 - 4.252E3/
1438	C5H11O2H-3=C5H11O-3+OH	9.45E+15	0	41600	REV/6.25E10 0.0E0 1.19E4/
1439	C5H11O-1=CH2O+PC4H9	5.66E+20	-2.247	24960	REV/7.5E10 0.0E0 1.19E4/
1440	C5H11O-2=CH3CHO+NC3H7	1.69E+22	-2.601	19550	REV/8.5E10 0.0E0 1.19E4/
1441	C5H11O-3=C2H5+C2H5CHO	1.24E+18	-1.199	18590	REV/4.52E12 0.0E0 0.0E0/
1442	C5H11O2-1=C5H11-1+O2	2.34E+20	-1.62	35830	REV/7.54E12 0.0E0 0.0E0/
1443	C5H11O2-2=C5H11-2+O2	7.09E+22	-2.287	38150	REV/7.54E12 0.0E0 0.0E0/
1444	C5H11O2-3=C5H11-3+O2	3.42E+22	-2.282	38150	REV/2.083E10 -1.06E-1 1.385E4/
1445	C5H11O2-1=C5H10OOH1-2	2.00E+11	0	26850	REV/2.604E9 -1.06E-1 7.85E3/
1446	C5H11O2-1=C5H10OOH1-3	2.50E+10	0	20850	REV/3.255E8 -1.06E-1 6.05E3/
1447	C5H11O2-1=C5H10OOH1-4	3.13E+09	0	19050	REV/1.379E9 -5.03E-1 1.009E4/
1448	C5H11O2-1=C5H10OOH1-5	5.86E+08	0	25550	REV/7.79E11 -5.17E-1 1.396E4/
1449	C5H11O2-2=C5H10OOH2-1	3.00E+11	0	29400	REV/2.698E10 -1.4E-1 1.39E4/
1450	C5H11O2-2=C5H10OOH2-3	2.00E+11	0	26850	REV/3.372E9 -1.4E-1 7.9E3/
1451	C5H11O2-2=C5H10OOH2-4	2.50E+10	0	20850	REV/1.217E10 -5.17E-1 6.91E3/
1452	C5H11O2-2=C5H10OOH2-5	4.69E+09	0	22350	REV/1.948E11 -5.17E-1 8.96E3/
1453	C5H11O2-3=C5H10OOH3-1	7.50E+10	0	24400	REV/5.396E10 -1.4E-1 1.39E4/
1454	C5H11O2-3=C5H10OOH3-2	4.00E+11	0	26850	REV/1.523E31 -6.66E0 2.051E4/
1455	C5H11O2-1=C5H10-1+HO2	5.04E+38	-8.11	40490	REV/2.039E34 -7.696E0 1.675E4/
1456	C5H11O2-2=C5H10-1+HO2	5.08E+42	-9.41	41490	REV/7.05E28 -5.795E0 1.86E4/
1457	C5H11O2-2=C5H10-2+HO2	5.04E+38	-8.11	40490	REV/1.41E29 -5.795E0 1.86E4/
1458	C5H11O2-3=C5H10-2+HO2	1.01E+39	-8.11	40490	
1459	C5H10OOH1-2=>C5H10O1-2+OH	6.00E+11	0	22000	
1460	C5H10OOH1-3=>C5H10O1-3+OH	7.50E+10	0	15250	
1461	C5H10OOH1-4=>C5H10O1-4+OH	9.38E+09	0	6000	
1462	C5H10OOH1-5=>C5H10O1-5+OH	1.17E+09	0	1800	
1463	C5H10OOH2-1=>C5H10O1-2+OH	6.00E+11	0	22000	
1464	C5H10OOH2-3=>C5H10O2-3+OH	6.00E+11	0	22000	
1465	C5H10OOH2-4=>C5H10O2-4+OH	7.50E+10	0	15250	
1466	C5H10OOH2-5=>C5H10O1-4+OH	9.38E+09	0	6000	
1467	C5H10OOH3-2=>C5H10O2-3+OH	6.00E+11	0	22000	
1468	C5H10OOH3-1=>C5H10O1-3+OH	7.50E+10	0	15250	
1469	C5H10O1-2+OH=>CH2CO+NC3H7+H2O	2.50E+12	0	0	
1470	C5H10O1-3+OH=>C2H4+C2H5CO+H2O	2.50E+12	0	0	
1471	C5H10O1-4+OH=>CH3COCH2+C2H4+H2O	2.50E+12	0	0	
1472	C5H10O1-5+OH=>CH2CH2CHO+C2H4+H2O	2.50E+12	0	0	
1473	C5H10O2-3+OH=>CH3CHCO+C2H5+H2O	2.50E+12	0	0	
1474	C5H10O2-4+OH=>CH3CO+C3H6+H2O	2.50E+12	0	0	
1475	C5H10O1-2+OH=>C2H3CHO+C2H5+H2O	2.50E+12	0	0	
1476	C5H10O1-3+OH=>HCO+C4H8-1+H2O	2.50E+12	0	0	
1477	C5H10O1-4+OH=>CH2CHO+C3H6+H2O	2.50E+12	0	0	

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Table B .1. (cont.)

1478	C5H10O1-5+OH=>CH2O+C4H71-3+H2O	2.50E+12	0	0	
1479	C5H10O2-3+OH=>C2H3COCH3+CH3+H2O	2.50E+12	0	0	
1480	C5H10O2-4+OH=>CH3CHO+C3H5-S+H2O	2.50E+12	0	0	
1481	C5H10O1-2+HO2=>CH2CO+NC3H7+H2O2	5.00E+12	0	17700	
1482	C5H10O1-3+HO2=>C2H4+C2H5CO+H2O2	5.00E+12	0	17700	
1483	C5H10O1-4+HO2=>CH3COCH2+C2H4+H2O2	5.00E+12	0	17700	
1484	C5H10O1-5+HO2=>CH2CH2CHO+C2H4+H2O2	5.00E+12	0	17700	
1485	C5H10O2-3+HO2=>CH3CHCO+C2H5+H2O2	5.00E+12	0	17700	
1486	C5H10O2-4+HO2=>CH3CO+C3H6+H2O2	5.00E+12	0	17700	
1487	C5H10O1-2+HO2=>C2H3CHO+C2H5+H2O2	5.00E+12	0	17700	
1488	C5H10O1-3+HO2=>HCO+C4H8-1+H2O2	5.00E+12	0	17700	
1489	C5H10O1-4+HO2=>CH2CHO+C3H6+H2O2	5.00E+12	0	17700	
1490	C5H10O1-5+HO2=>CH2O+C4H71-3+H2O2	5.00E+12	0	17700	
1491	C5H10O2-3+HO2=>C2H3COCH3+CH3+H2O2	5.00E+12	0	17700	
1492	C5H10O2-4+HO2=>CH3CHO+C3H5-S+H2O2	5.00E+12	0	17700	REV/1.0E11 0.0E0 1.1E4/
1493	C5H10OOH1-2=C5H10-1+HO2	3.45E+17	-1.556	17980	REV/1.0E11 0.0E0 1.175E4/
1494	C5H10OOH2-1=C5H10-1+HO2	6.46E+19	-2.231	21050	REV/1.0E11 0.0E0 1.175E4/
1495	C5H10OOH2-3=C5H10-2+HO2	9.65E+19	-2.455	20680	REV/1.0E11 0.0E0 1.175E4/
1496	C5H10OOH3-2=C5H10-2+HO2	9.65E+19	-2.455	20680	
1497	C5H10OOH1-3=>OH+CH2O+C4H8-1	8.28E+13	-0.17	30090	
1498	C5H10OOH2-4=>OH+CH3CHO+C3H6	8.31E+17	-1.4	27170	
1499	C5H10OOH3-1=>OH+C2H5CHO+C2H4	3.10E+18	-1.73	26820	REV/7.54E12 0.0E0 0.0E0/
1500	C5H10OOH1-2O2=C5H10OOH1-2+O2	8.04E+22	-2.295	37970	REV/7.54E12 0.0E0 0.0E0/
1501	C5H10OOH1-3O2=C5H10OOH1-3+O2	8.04E+22	-2.295	37970	REV/7.54E12 0.0E0 0.0E0/
1502	C5H10OOH1-4O2=C5H10OOH1-4+O2	8.04E+22	-2.295	37970	REV/4.52E12 0.0E0 0.0E0/
1503	C5H10OOH1-5O2=C5H10OOH1-5+O2	2.78E+20	-1.623	35690	REV/4.52E12 0.0E0 0.0E0/
1504	C5H10OOH2-1O2=C5H10OOH2-1+O2	2.57E+20	-1.62	35650	REV/7.54E12 0.0E0 0.0E0/
1505	C5H10OOH2-3O2=C5H10OOH2-3+O2	7.25E+22	-2.29	37910	REV/7.54E12 0.0E0 0.0E0/
1506	C5H10OOH2-4O2=C5H10OOH2-4+O2	7.25E+22	-2.29	37910	REV/4.52E12 0.0E0 0.0E0/
1507	C5H10OOH2-5O2=C5H10OOH2-5+O2	2.57E+20	-1.62	35650	REV/4.52E12 0.0E0 0.0E0/
1508	C5H10OOH3-1O2=C5H10OOH3-1+O2	2.57E+20	-1.62	35650	REV/7.54E12 0.0E0 0.0E0/
1509	C5H10OOH3-2O2=C5H10OOH3-2+O2	7.25E+22	-2.29	37910	REV/2.78E4 1.354E0 4.895E4/
1510	C5H10OOH1-2O2=NC5KET12+OH	2.00E+11	0	26400	REV/1.109E3 1.533E0 4.474E4/
1511	C5H10OOH1-3O2=NC5KET13+OH	2.50E+10	0	21400	REV/1.386E2 1.533E0 4.269E4/
1512	C5H10OOH1-4O2=NC5KET14+OH	3.13E+09	0	19350	REV/2.011E1 1.504E0 4.588E4/
1513	C5H10OOH1-5O2=NC5KET15+OH	3.91E+08	0	22550	REV/2.785E2 1.883E0 5.005E4/
1514	C5H10OOH2-1O2=NC5KET21+OH	1.00E+11	0	23850	REV/1.346E3 1.773E0 4.912E4/
1515	C5H10OOH2-3O2=NC5KET23+OH	1.00E+11	0	23850	REV/5.624E1 1.946E0 4.391E4/
1516	C5H10OOH2-4O2=NC5KET24+OH	1.25E+10	0	17850	REV/9.716E0 1.893E0 4.212E4/
1517	C5H10OOH2-5O2=NC5KET25+OH	1.56E+09	0	16050	REV/6.548E1 1.882E0 4.422E4/
1518	C5H10OOH3-1O2=NC5KET31+OH	1.25E+10	0	17850	REV/9.884E2 1.781E0 4.939E4/
1519	C5H10OOH3-2O2=NC5KET32+OH	1.00E+11	0	23850	
1520	NC5KET12=>NC3H7CHO+HCO+OH	1.05E+16	0	41600	
1521	NC5KET13=>C2H5CHO+CH2CHO+OH	1.05E+16	0	41600	

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Table B .1. (cont.)

1522	NC5KET14=>CH3CHO+CH2CH2CHO+OH	1.05E+16	0	41600	
1523	NC5KET15=>CH2O+C3H6CHO-1+OH	1.50E+16	0	42000	
1524	NC5KET21=>CH2O+NC3H7CO+OH	1.50E+16	0	42000	
1525	NC5KET23=>C2H5CHO+CH3CO+OH	1.50E+16	0	42000	
1526	NC5KET24=>CH3CHO+CH3COCH2+OH	1.50E+16	0	42000	
1527	NC5KET25=>CH2O+CH2CH2COCH3+OH	1.50E+16	0	42000	
1528	NC5KET31=>CH2O+C2H5COCH2+OH	1.50E+16	0	42000	
1529	NC5KET32=>CH3CHO+C2H5CO+OH	1.05E+16	0	41600	REV/4.75E12 0.0E0 -7.82E2/
1530	C5H10OH-1=C5H10-1+OH	1.50E+13	0	25830	REV/4.75E12 0.0E0 -7.82E2/
1531	C5H10OH-2=C5H10-2+OH	1.50E+13	0	25830	REV/2.0E12 0.0E0 0.0E0/
1532	O2C5H10OH-1=C5H10OH-1+O2	1.06E+21	-1.84	37750	
1533	O2C5H10OH-1=>NC3H7CHO+CH2O+OH	2.50E+10	0	18860	REV/2.0E12 0.0E0 0.0E0/
1534	O2C5H10OH-2=C5H10OH-2+O2	3.39E+21	-2.01	37870	
1535	O2C5H10OH-2=>C2H5CHO+CH3CHO+OH	2.50E+10	0	18860	REV/4.0E12 0.0E0 -5.96E2/
1536	NC6H14=C5H11-1+CH3	1.61E+22	-1.61	89350	REV/4.0E12 0.0E0 -5.96E2/
1537	NC6H14=2NC3H7	2.17E+24	-2.19	87840	REV/4.0E12 0.0E0 -5.96E2/
1538	NC6H14=PC4H9+C2H5	1.62E+24	-2.21	88580	REV/3.61E13 0.0E0 0.0E0/
1539	NC6H14=C6H13-1+H	1.36E+17	-0.36	101200	REV/3.61E13 0.0E0 0.0E0/
1540	NC6H14=C6H13-2+H	2.09E+18	-0.7	98710	REV/3.61E13 0.0E0 0.0E0/
1541	NC6H14=C6H13-3+H	2.09E+18	-0.7	98710	REV/1.998E1 3.38E0 8.615E3/
1542	NC6H14+H=C6H13-1+H2	1.88E+05	2.75	6280	REV/1.795E1 3.38E0 9.318E3/
1543	NC6H14+H=C6H13-2+H2	2.60E+06	2.4	4471	REV/1.795E1 3.38E0 9.318E3/
1544	NC6H14+H=C6H13-3+H2	2.60E+06	2.4	4471	REV/1.167E2 3.04E0 5.689E3/
1545	NC6H14+O=C6H13-1+OH	2.09E+06	2.42	4766	REV/4.308E0 3.4E0 6.281E3/
1546	NC6H14+O=C6H13-2+OH	1.19E+06	2.44	2846	REV/4.308E0 3.4E0 6.281E3/
1547	NC6H14+O=C6H13-3+OH	1.19E+06	2.44	2846	REV/2.906E4 2.33E0 1.818E4/
1548	NC6H14+OH=C6H13-1+H2O	2.57E+07	1.8	954	REV/3.599E2 2.87E0 1.914E4/
1549	NC6H14+OH=C6H13-2+H2O	4.90E+06	2	-596	REV/3.599E2 2.87E0 1.914E4/
1550	NC6H14+OH=C6H13-3+H2O	4.90E+06	2	-596	REV/8.77E-2 3.84E0 1.103E4/
1551	NC6H14+CH3=C6H13-1+CH4	9.04E-01	3.65	7154	REV/1.058E3 2.67E0 1.396E4/
1552	NC6H14+CH3=C6H13-3+CH4	1.68E+05	2.13	7574	REV/1.058E3 2.67E0 1.396E4/
1553	NC6H14+CH3=C6H13-2+CH4	1.68E+05	2.13	7574	REV/4.983E3 2.44E0 3.025E3/
1554	NC6H14+HO2=C6H13-1+H2O2	8.10E+04	2.5	16690	REV/4.699E2 2.78E0 3.709E3/
1555	NC6H14+HO2=C6H13-2+H2O2	1.18E+05	2.5	14860	REV/4.699E2 2.78E0 3.709E3/
1556	NC6H14+HO2=C6H13-3+H2O2	1.18E+05	2.5	14860	REV/1.2E10 0.0E0 9.2E3/
1557	NC6H14+CH3O=C6H13-1+CH3OH	3.16E+11	0	7000	REV/8.91E9 0.0E0 7.2E3/
1558	NC6H14+CH3O=C6H13-2+CH3OH	2.19E+11	0	5000	REV/8.91E9 0.0E0 7.2E3/
1559	NC6H14+CH3O=C6H13-3+CH3OH	2.19E+11	0	5000	REV/2.342E10 2.9E-1 4.51E2/
1560	NC6H14+O2=C6H13-1+HO2	4.20E+13	0	52800	REV/1.014E9 6.3E-1 3.13E2/
1561	NC6H14+O2=C6H13-2+HO2	2.80E+13	0	50160	REV/1.014E9 6.3E-1 3.13E2/
1562	NC6H14+O2=C6H13-3+HO2	2.80E+13	0	50160	REV/3.24E11 0.0E0 1.23E4/

(cont. on next page)

Table B .1. (cont.)

1563	NC6H14+C2H5=C6H13-1+C2H6	1.00E+11	0	13400	REV/1.0E11 0.0E0 1.29E4/
1564	NC6H14+C2H5=C6H13-2+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
1565	NC6H14+C2H5=C6H13-3+C2H6	1.00E+11	0	10400	REV/2.57E12 0.0E0 2.54E4/
1566	NC6H14+C2H3=C6H13-1+C2H4	1.00E+12	0	18000	REV/2.0E12 0.0E0 2.42E4/
1567	NC6H14+C2H3=C6H13-2+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
1568	NC6H14+C2H3=C6H13-3+C2H4	8.00E+11	0	16800	REV/9.695E4 2.0E0 1.43E3/
1569	NC6H14+CH3O2=C6H13-1+CH3O2H	8.10E+04	2.5	16690	REV/9.141E3 2.34E0 2.114E3/
1570	NC6H14+CH3O2=C6H13-2+CH3O2H	1.18E+05	2.5	14860	REV/9.141E3 2.34E0 2.114E3/
1571	NC6H14+CH3O2=C6H13-3+CH3O2H	1.18E+05	2.5	14860	REV/5.692E2 2.3E0 3.06E3/
1572	NC6H14+O2CHO=C6H13-1+HO2CHO	1.68E+13	0	20440	REV/2.464E1 2.64E0 2.823E3/
1573	NC6H14+O2CHO=C6H13-2+HO2CHO	1.12E+13	0	17690	REV/2.464E1 2.64E0 2.823E3/
1574	NC6H14+O2CHO=C6H13-3+HO2CHO	1.12E+13	0	17690	REV/1.44E10 0.0E0 1.5E4/
1575	C6H13O2-1+NC6H14=C6H13O2H-1+C6H13-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1576	C6H13O2-2+NC6H14=C6H13O2H-2+C6H13-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1577	C6H13O2-3+NC6H14=C6H13O2H-3+C6H13-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1578	C6H13O2-1+NC6H14=C6H13O2H-1+C6H13-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1579	C6H13O2-2+NC6H14=C6H13O2H-2+C6H13-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1580	C6H13O2-3+NC6H14=C6H13O2H-3+C6H13-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1581	C6H13O2-1+NC6H14=C6H13O2H-1+C6H13-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1582	C6H13O2-2+NC6H14=C6H13O2H-2+C6H13-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1583	C6H13O2-3+NC6H14=C6H13O2H-3+C6H13-3	8.06E+12	0	17700	REV/1.5E11 0.0E0 1.23E4/
1584	NC6H14+C6H13-1=NC6H14+C6H13-2	1.00E+11	0	10400	REV/1.5E11 0.0E0 1.23E4/
1585	NC6H14+C6H13-1=NC6H14+C6H13-3	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.04E4/
1586	NC6H14+C6H13-2=NC6H14+C6H13-3	1.00E+11	0	10400	REV/3.266E15 -5.6E-1 2.615E4/
1587	C6H13-1+HO2=C6H13O-1+OH	7.00E+12	0	-1000	REV/3.073E17 -1.15E0 2.807E4/
1588	C6H13-2+HO2=C6H13O-2+OH	7.00E+12	0	-1000	REV/3.073E17 -1.15E0 2.807E4/
1589	C6H13-3+HO2=C6H13O-3+OH	7.00E+12	0	-1000	REV/2.043E14 -2.6E-1 3.039E4/
1590	C6H13-1+CH3O2=C6H13O-1+CH3O	7.00E+12	0	-1000	REV/1.922E16 -8.5E-1 3.231E4/
1591	C6H13-2+CH3O2=C6H13O-2+CH3O	7.00E+12	0	-1000	REV/1.922E16 -8.5E-1 3.231E4/
1592	C6H13-3+CH3O2=C6H13O-3+CH3O	7.00E+12	0	-1000	REV/2.0E-19 0.0E0 1.75E4/
1593	C6H13-1+O2=C6H12-1+HO2	3.00E-19	0	3000	REV/2.0E-19 0.0E0 1.75E4/
1594	C6H13-2+O2=C6H12-1+HO2	4.50E-19	0	5020	REV/2.0E-19 0.0E0 1.75E4/
1595	C6H13-2+O2=C6H12-2+HO2	3.00E-19	0	3000	REV/2.0E-19 0.0E0 1.75E4/
1596	C6H13-3+O2=C6H12-2+HO2	3.00E-19	0	3000	REV/2.0E-19 0.0E0 1.75E4/
1597	C6H13-3+O2=C6H12-3+HO2	3.00E-19	0	3000	REV/3.3E11 0.0E0 7.2E3/
1598	C6H13-1=C2H4+PC4H9	6.39E+19	-1.97	30640	REV/1.0E13 0.0E0 2.9E3/
1599	C6H13-1=C6H12-1+H	9.62E+13	-0.26	36000	REV/1.5E11 0.0E0 7.2E3/
1600	C6H13-2=C3H6+NC3H7	1.83E+19	-1.8	30170	REV/1.0E13 0.0E0 1.2E3/
1601	C6H13-2=C6H12-1+H	6.25E+12	0.09	36820	REV/1.0E13 0.0E0 2.9E3/
1602	C6H13-2=C6H12-2+H	1.27E+13	-0.09	35650	REV/1.5E11 0.0E0 7.2E3/
1603	C6H13-3=C4H8-1+C2H5	1.20E+19	-1.76	30450	REV/1.5E11 0.0E0 7.2E3/
1604	C6H13-3=C5H10-1+CH3	1.67E+16	-0.93	31480	REV/1.0E13 0.0E0 2.9E3/
1605	C6H13-3=C6H12-2+H	1.27E+13	-0.09	35650	REV/1.0E13 0.0E0 2.9E3/
1606	C6H13-3=C6H12-3+H	4.66E+12	-0.02	35740	REV/3.558E7 1.97E0 4.127E4/

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Table B .1. (cont.)

1607	C6H13-1=C6H13-2	5.48E+08	1.62	38760	REV/9.709E7 1.31E0 3.627E4/
1608	C6H13-1=C6H13-3	1.50E+09	0.97	33760	REV/1.0E13 0.0E0 0.0E0/
1609	C6H12-1=NC3H7+C3H5-A	1.00E+16	0	71000	REV/1.0E13 0.0E0 0.0E0/
1610	C6H12-2=C2H5+C4H71-3	1.00E+16	0	71000	REV/1.0E13 0.0E0 0.0E0/
1611	C6H12-3=CH3+C5H91-3	1.00E+16	0	71000	
1612	C6H12-1+OH=>C5H11-1+CH2O	1.00E+11	0	-4000	
1613	C6H12-2+OH=>PC4H9+CH3CHO	1.00E+11	0	-4000	
1614	C6H12-3+OH=>PC4H9+CH3CHO	1.00E+11	0	-4000	
1615	C6H12-1+O=>C5H11-1+HCO	1.00E+11	0	-1050	
1616	C6H12-2+O=>PC4H9+CH3CO	1.00E+11	0	-1050	REV/4.378E6 2.1E0 2.033E4/
1617	C6H12-1+H=C6H111-3+H2	3.38E+05	2.36	207	REV/3.896E3 2.74E0 1.125E4/
1618	C6H12-1+H=C6H111-4+H2	1.30E+06	2.4	4471	REV/3.896E3 2.74E0 1.125E4/
1619	C6H12-1+H=C6H111-5+H2	1.30E+06	2.4	4471	REV/3.12E4 2.54E0 1.103E4/
1620	C6H12-1+H=C6H111-6+H2	6.65E+05	2.54	6756	REV/1.552E6 2.38E0 3.336E4/
1621	C6H12-1+OH=C6H111-3+H2O	2.76E+04	2.64	-1919	REV/6.06E5 1.95E0 2.19E4/
1622	C6H12-1+OH=C6H111-4+H2O	4.67E+07	1.61	-35	REV/6.06E5 1.95E0 2.19E4/
1623	C6H12-1+OH=C6H111-5+H2O	4.67E+07	1.61	-35	REV/1.071E9 9.7E-1 2.101E4/
1624	C6H12-1+OH=C6H111-6+H2O	5.27E+09	0.97	1586	REV/1.25E3 3.05E0 2.46E4/
1625	C6H12-1+CH3=C6H111-3+CH4	3.69E+00	3.31	4002	REV/1.182E-1 3.8E0 1.274E4/
1626	C6H12-1+CH3=C6H111-4+CH4	1.51E+00	3.46	5481	REV/1.182E-1 3.8E0 1.274E4/
1627	C6H12-1+CH3=C6H111-5+CH4	1.51E+00	3.46	5481	REV/5.541E-1 3.65E0 1.19E4/
1628	C6H12-1+CH3=C6H111-6+CH4	4.52E-01	3.65	7154	
1629	C6H12-1+HO2=C6H111-3+H2O2	9.64E+03	2.55	10530	
1630	C6H12-1+HO2=C6H111-4+H2O2	9.64E+03	2.6	13910	
1631	C6H12-1+HO2=C6H111-5+H2O2	9.64E+03	2.6	13910	
1632	C6H12-1+HO2=C6H111-6+H2O2	2.38E+04	2.55	16490	REV/3.345E6 1.79E0 1.132E4/
1633	C6H12-1+CH3O2=C6H111-3+CH3O2H	4.82E+03	2.55	10530	REV/1.546E3 2.44E0 1.362E3/
1634	C6H12-1+CH3O2=C6H111-4+CH3O2H	9.64E+03	2.6	13910	REV/1.546E3 2.44E0 1.362E3/
1635	C6H12-1+CH3O2=C6H111-5+CH3O2H	9.64E+03	2.6	13910	REV/5.976E4 2.04E0 1.436E3/
1636	C6H12-1+CH3O2=C6H111-6+CH3O2H	2.38E+04	2.55	16490	REV/2.501E2 2.67E0 2.7E4/
1637	C6H12-1+CH3O=C6H111-3+CH3OH	4.00E+01	2.9	8609	REV/2.095E8 3.7E-1 9.621E3/
1638	C6H12-1+CH3O=C6H111-4+CH3OH	1.45E+11	0	4571	REV/2.095E8 3.7E-1 9.621E3/
1639	C6H12-1+CH3O=C6H111-5+CH3OH	1.45E+11	0	4571	REV/4.908E9 2.0E-2 8.998E3/
1640	C6H12-1+CH3O=C6H111-6+CH3OH	2.17E+11	0	6458	REV/4.563E6 2.06E0 1.974E4/
1641	C6H12-2+H=C6H111-3+H2	1.73E+05	2.5	2492	REV/4.384E6 2.1E0 2.033E4/
1642	C6H12-2+H=C6H112-4+H2	3.38E+05	2.36	207	REV/3.921E3 2.74E0 1.125E4/
1643	C6H12-2+H=C6H112-5+H2	1.30E+06	2.4	4471	REV/3.122E4 2.53E0 1.103E4/
1644	C6H12-2+H=C6H112-6+H2	6.65E+05	2.54	6756	REV/3.563E8 1.56E0 3.211E4/
1645	C6H12-2+OH=C6H111-3+H2O	3.12E+06	2	-298	REV/1.554E6 2.38E0 3.336E4/
1646	C6H12-2+OH=C6H112-4+H2O	2.76E+04	2.64	-1919	REV/6.099E3 1.95E0 2.19E4/

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Table B .1. (cont.)

1647	C6H12-2+OH=C6H112-5+H2O	4.67E+05	1.61	-35	REV/1.071E9 9.6E-1 2.101E4/
1648	C6H12-2+OH=C6H112-6+H2O	5.27E+09	0.97	1586	REV/1.523E3 3.06E0 2.341E4/
1649	C6H12-2+CH3=C6H111-3+CH4	2.21E+00	3.5	5675	REV/1.252E3 3.05E0 2.46E4/
1650	C6H12-2+CH3=C6H112-4+CH4	3.69E+00	3.31	4002	REV/1.19E-1 3.8E0 1.274E4/
1651	C6H12-2+CH3=C6H112-5+CH4	1.51E+00	3.46	5481	REV/5.543E-1 3.64E0 1.19E4/
1652	C6H12-2+CH3=C6H112-6+CH4	4.52E-01	3.65	7154	REV/6.534E6 1.84E0 1.485E4/
1653	C6H12-2+HO2=C6H111-3+H2O2	9.64E+03	2.6	13910	REV/1.609E6 1.96E0 1.434E4/
1654	C6H12-2+HO2=C6H112-4+H2O2	4.82E+03	2.55	10530	REV/7.473E2 2.61E0 4.382E3/
1655	C6H12-2+HO2=C6H112-5+H2O2	9.64E+03	2.6	13910	REV/2.871E4 2.22E0 4.456E3/
1656	C6H12-2+HO2=C6H112-6+H2O2	2.38E+04	2.55	16490	REV/1.361E7 1.66E0 1.183E4/
1657	C6H12-2+CH3O2=C6H111-3+CH3O2H	9.64E+03	2.6	13910	REV/3.35E6 1.79E0 1.132E4/
1658	C6H12-2+CH3O2=C6H112-4+CH3O2H	4.82E+03	2.55	10530	REV/1.556E3 2.44E0 1.362E3/
1659	C6H12-2+CH3O2=C6H112-5+CH3O2H	9.64E+03	2.6	13910	REV/5.978E4 2.04E0 1.436E3/
1660	C6H12-2+CH3O2=C6H112-6+CH3O2H	2.38E+04	2.55	16490	REV/1.144E3 2.54E0 2.751E4/
1661	C6H12-2+CH3O=C6H111-3+CH3OH	9.00E+01	2.95	11990	REV/2.504E2 2.66E0 2.7E4/
1662	C6H12-2+CH3O=C6H112-4+CH3OH	4.00E+01	2.9	8609	REV/2.109E8 3.7E-1 9.621E3/
1663	C6H12-2+CH3O=C6H112-5+CH3OH	1.45E+11	0	4571	REV/4.91E9 2.0E-2 8.998E3/
1664	C6H12-2+CH3O=C6H112-6+CH3OH	2.17E+11	0	6458	REV/3.078E4 2.54E0 1.103E4/
1665	C6H12-3+H=C6H113-1+H2	1.33E+06	2.54	6756	REV/3.215E6 2.17E0 2.042E4/
1666	C6H12-3+H=C6H112-4+H2	6.75E+05	2.36	207	REV/1.056E9 9.7E-1 2.101E4/
1667	C6H12-3+OH=C6H113-1+H2O	1.05E+10	0.97	1586	REV/1.14E6 2.45E0 3.345E4/
1668	C6H12-3+OH=C6H112-4+H2O	5.53E+04	2.64	-1919	REV/5.467E-1 3.65E0 1.19E4/
1669	C6H12-3+CH3=C6H113-1+CH4	9.04E-01	3.65	7154	REV/9.179E2 3.12E0 2.469E4/
1670	C6H12-3+CH3=C6H112-4+CH4	7.38E+00	3.31	4002	REV/2.832E4 2.22E0 4.456E3/
1671	C6H12-3+HO2=C6H113-1+H2O2	4.76E+04	2.55	16490	REV/1.18E6 2.03E0 1.443E4/
1672	C6H12-3+HO2=C6H112-4+H2O2	9.64E+03	2.55	10530	REV/5.896E4 2.04E0 1.436E3/
1673	C6H12-3+CH3O2=C6H113-1+CH3O2H	4.76E+04	2.55	16490	REV/2.456E6 1.85E0 1.141E4/
1674	C6H12-3+CH3O2=C6H112-4+CH3O2H	9.64E+03	2.55	10530	REV/4.843E9 2.0E-2 8.998E3/
1675	C6H12-3+CH3O=C6H113-1+CH3OH	4.34E+11	0	6458	REV/1.836E2 2.73E0 2.709E4/
1676	C6H12-3+CH3O=C6H112-4+CH3OH	8.00E+01	2.9	8609	REV/1.07E16 -1.14E0 1.58E4/
1677	C6H111-3+HO2=C6H11O1-3+OH	9.64E+12	0	0	REV/1.045E18 -1.72E0 2.057E4/
1678	C6H111-3+CH3O2=C6H11O1-3+CH3O	9.64E+12	0	0	REV/6.844E14 -8.0E-1 1.841E4/
1679	C6H111-3+C2H5O2=C6H11O1-3+C2H5O	9.64E+12	0	0	REV/3.076E14 -2.5E-1 4.755E4/
1680	C6H111-6=C6H111-3	1.11E+12	0	31700	REV/9.704E15 -1.13E0 1.579E4/
1681	C6H112-4+HO2=C6H11O2-4+OH	9.64E+12	0	0	REV/9.478E17 -1.71E0 2.056E4/
1682	C6H112-4+CH3O2=C6H11O2-4+CH3O	9.64E+12	0	0	REV/6.204E14 -7.8E-1 1.84E4/

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Table B .1. (cont.)

1683	C6H112-4+C2H5O2=C6H11O2-4+C2H5O	9.64E+12	0	0	REV/1.0E11 0.0E0 9.6E3/
1684	C6H11O1-3=C2H3CHO+NC3H7	1.43E+20	-2.04	11230	REV/1.0E11 0.0E0 9.6E3/
1685	C6H11O1-3=NC3H7CHO+C2H3	2.40E+18	-1.63	23410	REV/1.0E11 0.0E0 9.6E3/
1686	C6H11O2-4=SC3H5CHO+C2H5	5.45E+19	-1.92	10760	REV/1.0E11 0.0E0 9.6E3/
1687	C6H11O2-4=C2H5CHO+C3H5-S	2.35E+22	-2.58	29310	REV/4.52E12 0.0E0 0.0E0/
1688	C6H13O2-1=C6H13-1+O2	5.15E+20	-1.71	35790	REV/7.54E12 0.0E0 0.0E0/
1689	C6H13O2-2=C6H13-2+O2	2.18E+23	-2.33	38040	REV/7.54E12 0.0E0 0.0E0/
1690	C6H13O2-3=C6H13-3+O2	2.18E+23	-2.33	38040	REV/9.781E13 -2.1E-1 2.984E4/
1691	C6H13-1+C6H13O2-1=2C6H13O-1	7.00E+12	0	-1000	REV/3.628E13 -1.7E-1 2.95E4/
1692	C6H13-1+C6H13O2-2=C6H13O-1+C6H13O-2	7.00E+12	0	-1000	REV/3.628E13 -1.7E-1 2.95E4/
1693	C6H13-1+C6H13O2-3=C6H13O-1+C6H13O-3	7.00E+12	0	-1000	REV/9.205E15 -7.9E-1 3.176E4/
1694	C6H13-2+C6H13O2-1=C6H13O-2+C6H13O-1	7.00E+12	0	-1000	REV/3.414E15 -7.6E-1 3.142E4/
1695	C6H13-2+C6H13O2-2=2C6H13O-2	7.00E+12	0	-1000	REV/3.414E15 -7.6E-1 3.142E4/
1696	C6H13-2+C6H13O2-3=C6H13O-2+C6H13O-3	7.00E+12	0	-1000	REV/9.205E15 -7.9E-1 3.176E4/
1697	C6H13-3+C6H13O2-1=C6H13O-3+C6H13O-1	7.00E+12	0	-1000	REV/3.414E15 -7.6E-1 3.142E4/
1698	C6H13-3+C6H13O2-2=C6H13O-3+C6H13O-2	7.00E+12	0	-1000	REV/3.414E15 -7.6E-1 3.142E4/
1699	C6H13-3+C6H13O2-3=2C6H13O-3	7.00E+12	0	-1000	REV/9.638E29 -6.22E0 2.047E4/
1700	C6H13O2-1=C6H12-1+HO2	5.04E+38	-8.11	40490	REV/5.885E32 -7.24E0 1.67E4/
1701	C6H13O2-2=C6H12-1+HO2	5.08E+42	-9.41	41490	REV/2.876E28 -5.77E0 1.857E4/
1702	C6H13O2-2=C6H12-2+HO2	5.04E+38	-8.11	40490	REV/1.569E29 -5.83E0 1.848E4/
1703	C6H13O2-3=C6H12-3+HO2	1.01E+39	-8.11	40490	REV/2.402E10 -1.2E-1 1.386E4/
1704	C6H13O2-1=C6H12OOH1-2	2.00E+11	0	26850	REV/3.003E9 -1.2E-1 7.86E3/
1705	C6H13O2-1=C6H12OOH1-3	2.50E+10	0	20850	REV/3.754E8 -1.2E-1 6.06E3/
1706	C6H13O2-1=C6H12OOH1-4	3.13E+09	0	19050	REV/4.692E7 -1.2E-1 9.06E3/
1707	C6H13O2-1=C6H12OOH1-5	3.91E+08	0	22050	REV/7.948E11 -5.2E-1 1.395E4/
1708	C6H13O2-2=C6H12OOH2-1	3.00E+11	0	29400	REV/2.578E10 -1.3E-1 1.388E4/
1709	C6H13O2-2=C6H12OOH2-3	2.00E+11	0	26850	REV/3.223E9 -1.3E-1 7.88E3/
1710	C6H13O2-2=C6H12OOH2-4	2.50E+10	0	20850	REV/4.028E8 -1.3E-1 6.08E3/
1711	C6H13O2-2=C6H12OOH2-5	3.13E+09	0	19050	REV/1.553E9 -5.2E-1 1.01E4/
1712	C6H13O2-2=C6H12OOH2-6	5.86E+08	0	25550	REV/9.935E10 -5.2E-1 8.95E3/
1713	C6H13O2-3=C6H12OOH3-1	3.75E+10	0	24400	REV/2.578E10 -1.3E-1 1.388E4/
1714	C6H13O2-3=C6H12OOH3-2	2.00E+11	0	26850	REV/2.578E10 -1.3E-1 1.388E4/
1715	C6H13O2-3=C6H12OOH3-4	2.00E+11	0	26850	REV/3.223E9 -1.3E-1 7.88E3/
1716	C6H13O2-3=C6H12OOH3-5	2.50E+10	0	20850	REV/1.242E10 -5.2E-1 6.9E3/
1717	C6H13O2-3=C6H12OOH3-6	4.69E+09	0	22350	REV/3.538E13 -7.8E-1 3.36E4/
1718	C6H13O2-1+HO2=C6H13O2H-1+O2	1.75E+10	0	-3275	REV/4.447E13 -8.1E-1 3.364E4/
1719	C6H13O2-2+HO2=C6H13O2H-2+O2	1.75E+10	0	-3275	REV/4.447E13 -8.1E-1 3.364E4/
1720	C6H13O2-3+HO2=C6H13O2H-3+O2	1.75E+10	0	-3275	REV/2.4E12 0.0E0 1.0E4/

(cont. on next page)

Table B .1. (cont.)

1721	C6H13O2-1+H2O2=C6H13O2H-1+HO2	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
1722	C6H13O2-2+H2O2=C6H13O2H-2+HO2	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
1723	C6H13O2-3+H2O2=C6H13O2H-3+HO2	2.40E+12	0	10000	
1724	C6H13O2-1+CH3O2=>C6H13O-1+CH3O+O2	1.40E+16	-1.61	1860	
1725	C6H13O2-2+CH3O2=>C6H13O-2+CH3O+O2	1.40E+16	-1.61	1860	
1726	C6H13O2-3+CH3O2=>C6H13O-3+CH3O+O2	1.40E+16	-1.61	1860	
1727	2C6H13O2-1=>O2+2C6H13O-1	1.40E+16	-1.61	1860	
1728	C6H13O2-1+C6H13O2-2=>O2+C6H13O-1+C6H13O-2	1.40E+16	-1.61	1860	
1729	C6H13O2-1+C6H13O2-3=>O2+C6H13O-1+C6H13O-3	1.40E+16	-1.61	1860	
1730	2C6H13O2-2=>O2+2C6H13O-2	1.40E+16	-1.61	1860	
1731	C6H13O2-2+C6H13O2-3=>O2+C6H13O-2+C6H13O-3	1.40E+16	-1.61	1860	
1732	2C6H13O2-3=>O2+2C6H13O-3	1.40E+16	-1.61	1860	REV/2.025E7 1.93E0 -6.512E3/
1733	C6H13O2H-1=C6H13O-1+OH	1.00E+16	0	39000	REV/5.977E6 2.0E0 -6.892E3/
1734	C6H13O2H-2=C6H13O-2+OH	1.00E+16	0	39000	REV/5.977E6 2.0E0 -6.892E3/
1735	C6H13O2H-3=C6H13O-3+OH	1.00E+16	0	39000	REV/1.0E11 0.0E0 1.19E4/
1736	C6H13O-1=C5H11-1+CH2O	5.23E+20	-2.08	24830	REV/1.0E11 0.0E0 1.19E4/
1737	C6H13O-2=PC4H9+CH3CHO	2.37E+22	-2.61	19620	REV/1.0E11 0.0E0 1.19E4/
1738	C6H13O-3=C2H5CHO+NC3H7	8.05E+17	-1.17	18170	
1739	C6H12OOH1-2=>C6H12O1-2+OH	6.00E+11	0	22000	
1740	C6H12OOH1-3=>C6H12O1-3+OH	7.50E+10	0	15250	
1741	C6H12OOH1-4=>C6H12O1-4+OH	9.38E+09	0	7000	
1742	C6H12OOH1-5=>C6H12O1-5+OH	1.17E+09	0	1800	
1743	C6H12OOH2-1=>C6H12O1-2+OH	6.00E+11	0	22000	
1744	C6H12OOH2-3=>C6H12O2-3+OH	6.00E+11	0	22000	
1745	C6H12OOH2-4=>C6H12O2-4+OH	7.50E+10	0	15250	
1746	C6H12OOH2-5=>C6H12O2-5+OH	9.38E+09	0	7000	
1747	C6H12OOH2-6=>C6H12O1-5+OH	1.17E+09	0	1800	
1748	C6H12OOH3-2=>C6H12O2-3+OH	6.00E+11	0	22000	
1749	C6H12OOH3-4=>C6H12O3-4+OH	6.00E+11	0	22000	
1750	C6H12OOH3-1=>C6H12O1-3+OH	7.50E+10	0	15250	
1751	C6H12OOH3-5=>C6H12O2-4+OH	7.50E+10	0	15250	
1752	C6H12OOH3-6=>C6H12O1-4+OH	9.38E+09	0	7000	
1753	C6H12OOH1-3=>OH+CH2O+C5H10-1	7.70E+13	-0.16	30090	
1754	C6H12OOH2-4=>OH+CH3CHO+C4H8-1	2.93E+18	-1.7	24080	
1755	C6H12OOH3-5=>OH+C2H5CHO+C3H6	1.17E+17	-1.31	28880	
1756	C6H12OOH3-1=>OH+CH3CHO+2C2H4	7.33E+18	-1.74	27420	REV/7.54E12 0.0E0 0.0E0/
1757	C6H12OOH1-2O2=C6H12OOH1-2+O2	8.87E+22	-2.31	37980	REV/7.54E12 0.0E0 0.0E0/
1758	C6H12OOH1-3O2=C6H12OOH1-3+O2	8.87E+22	-2.31	37980	REV/7.54E12 0.0E0 0.0E0/
1759	C6H12OOH1-4O2=C6H12OOH1-4+O2	8.87E+22	-2.31	37980	REV/7.54E12 0.0E0 0.0E0/
1760	C6H12OOH1-5O2=C6H12OOH1-5+O2	8.87E+22	-2.31	37980	REV/4.52E12 0.0E0 0.0E0/
1761	C6H12OOH2-1O2=C6H12OOH2-1+O2	1.46E+20	-1.64	35670	REV/7.54E12 0.0E0 0.0E0/
1762	C6H12OOH2-3O2=C6H12OOH2-3+O2	4.79E+22	-2.33	37960	REV/7.54E12 0.0E0 0.0E0/
1763	C6H12OOH2-4O2=C6H12OOH2-4+O2	4.79E+22	-2.33	37960	REV/7.54E12 0.0E0 0.0E0/
1764	C6H12OOH2-5O2=C6H12OOH2-5+O2	4.79E+22	-2.33	37960	REV/4.52E12 0.0E0 0.0E0/
1765	C6H12OOH2-6O2=C6H12OOH2-6+O2	1.46E+20	-1.64	35670	REV/4.52E12 0.0E0 0.0E0/
1766	C6H12OOH3-1O2=C6H12OOH3-1+O2	1.46E+20	-1.64	35670	REV/7.54E12 0.0E0 0.0E0/
1767	C6H12OOH3-2O2=C6H12OOH3-2+O2	4.79E+22	-2.33	37960	REV/7.54E12 0.0E0 0.0E0/

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Table B .1. (cont.)

1768	C6H12OOH3-4O2=C6H12OOH3-4+O2	4.79E+22	-2.33	37960	REV/7.54E12 0.0E0 0.0E0/
1769	C6H12OOH3-5O2=C6H12OOH3-5+O2	4.79E+22	-2.33	37960	REV/4.52E12 0.0E0 0.0E0/
1770	C6H12OOH3-6O2=C6H12OOH3-6+O2	1.46E+20	-1.64	35670	REV/2.607E-12 6.14E0 3.97E4/
1771	C6H12OOH1-2O2=NC6KET12+OH	2.00E+11	0	26400	REV/8.825E2 1.56E0 4.471E4/
1772	C6H12OOH1-3O2=NC6KET13+OH	2.50E+10	0	21400	REV/1.103E2 1.56E0 4.266E4/
1773	C6H12OOH1-4O2=NC6KET14+OH	3.13E+09	0	19350	REV/1.379E1 1.56E0 4.586E4/
1774	C6H12OOH1-5O2=NC6KET15+OH	3.91E+08	0	22550	REV/2.253E2 1.91E0 5.003E4/
1775	C6H12OOH2-1O2=NC6KET21+OH	1.00E+11	0	23850	REV/1.156E3 1.79E0 4.909E4/
1776	C6H12OOH2-3O2=NC6KET23+OH	1.00E+11	0	23850	REV/4.618E1 1.97E0 4.388E4/
1777	C6H12OOH2-4O2=NC6KET24+OH	1.25E+10	0	17850	REV/5.774E0 1.97E0 4.208E4/
1778	C6H12OOH2-5O2=NC6KET25+OH	1.56E+09	0	16050	REV/1.939E0 1.92E0 4.859E4/
1779	C6H12OOH2-6O2=NC6KET26+OH	3.91E+08	0	22550	REV/5.308E1 1.91E0 4.419E4/
1780	C6H12OOH3-1O2=NC6KET31+OH	1.25E+10	0	17850	REV/7.384E2 1.82E0 4.935E4/
1781	C6H12OOH3-2O2=NC6KET32+OH	1.00E+11	0	23850	REV/7.384E2 1.82E0 4.935E4/
1782	C6H12OOH3-4O2=NC6KET34+OH	1.00E+11	0	23850	REV/3.503E1 1.98E0 4.416E4/
1783	C6H12OOH3-5O2=NC6KET35+OH	1.25E+10	0	17850	REV/6.638E0 1.91E0 4.239E4/
1784	C6H12OOH3-6O2=NC6KET36+OH	1.56E+09	0	16050	
1785	NC6KET12=>NC4H9CHO+HCO+OH	1.00E+16	0	39000	
1786	NC6KET13=>NC3H7CHO+CH2CHO+OH	1.00E+16	0	39000	
1787	NC6KET14=>C2H5CHO+CH2CH2CHO+OH	1.00E+16	0	39000	
1788	NC6KET15=>CH3CHO+C3H6CHO-1+OH	1.00E+16	0	39000	
1789	NC6KET21=>CH2O+NC4H9CO+OH	1.00E+16	0	39000	
1790	NC6KET23=>NC3H7CHO+CH3CO+OH	1.00E+16	0	39000	
1791	NC6KET24=>C2H5CHO+CH3COCH2+OH	1.00E+16	0	39000	
1792	NC6KET25=>CH3CHO+CH2CH2COCH3+OH	1.00E+16	0	39000	
1793	NC6KET26=>CH2O+C3H6COCH3-1+OH	1.00E+16	0	39000	
1794	NC6KET31=>CH2O+NC3H7COCH2+OH	1.00E+16	0	39000	
1795	NC6KET32=>CH3CHO+NC3H7CO+OH	1.00E+16	0	39000	
1796	NC6KET34=>C2H5CHO+C2H5CO+OH	1.00E+16	0	39000	
1797	NC6KET35=>CH3CHO+C2H5COCH2+OH	1.00E+16	0	39000	
1798	NC6KET36=>CH2O+C2H5COC2H4P+OH	1.00E+16	0	39000	
1799	C6H12O1-2+OH=>C2H3CHO+NC3H7+H2O	2.50E+12	0	0	
1800	C6H12O1-3+OH=>C5H10-1+HCO+H2O	2.50E+12	0	0	
1801	C6H12O1-4+OH=>C4H8-1+CH2CHO+H2O	2.50E+12	0	0	
1802	C6H12O1-5+OH=>C3H6+CH2CH2CHO+H2O	2.50E+12	0	0	
1803	C6H12O2-3+OH=>C2H3COCH3+C2H5+H2O	2.50E+12	0	0	
1804	C6H12O2-4+OH=>C4H8-1+CH3CO+H2O	2.50E+12	0	0	
1805	C6H12O2-5+OH=>C3H6+CH3COCH2+H2O	2.50E+12	0	0	
1806	C6H12O3-4+OH=>C2H5COC2H3+CH3+H2O	2.50E+12	0	0	
1807	C6H12O1-2+OH=>CH2CO+PC4H9+H2O	2.50E+12	0	0	
1808	C6H12O1-3+OH=>C2H4+NC3H7CO+H2O	2.50E+12	0	0	
1809	C6H12O1-4+OH=>C2H4+C2H5COCH2+H2O	2.50E+12	0	0	
1810	C6H12O1-5+OH=>C2H4+CH2CH2COCH3+H2O	2.50E+12	0	0	

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Table B .1. (cont.)

1811	C6H12O2-3+OH=>CH3CHCO+NC3H7+H2O	2.50E+12	0	0	
1812	C6H12O2-4+OH=>C3H6+C2H5CO+H2O	2.50E+12	0	0	
1813	C6H12O2-5+OH=>CH3CHO+C4H71-3+H2O	2.50E+12	0	0	
1814	C6H12O3-4+OH=>C2H5CHO+C3H5-S+H2O	2.50E+12	0	0	
1815	C6H12O1-2+HO2=>C2H3CHO+NC3H7+H2O2	5.00E+12	0	17700	
1816	C6H12O1-3+HO2=>C5H10-1+HCO+H2O2	5.00E+12	0	17700	
1817	C6H12O1-4+HO2=>C4H8-1+CH2CHO+H2O2	5.00E+12	0	17700	
1818	C6H12O1-5+HO2=>C3H6+CH2CH2CHO+H2O2	5.00E+12	0	17700	
1819	C6H12O2-3+HO2=>C2H3COCH3+C2H5+H2O2	5.00E+12	0	17700	
1820	C6H12O2-4+HO2=>C4H8-1+CH3CO+H2O2	5.00E+12	0	17700	
1821	C6H12O2-5+HO2=>C3H6+CH3COCH2+H2O2	5.00E+12	0	17700	
1822	C6H12O3-4+HO2=>C2H5COC2H3+CH3+H2O2	5.00E+12	0	17700	
1823	C6H12O1-2+HO2=>CH2CO+PC4H9+H2O2	5.00E+12	0	17700	
1824	C6H12O1-3+HO2=>C2H4+NC3H7CO+H2O2	5.00E+12	0	17700	
1825	C6H12O1-4+HO2=>C2H4+C2H5COCH2+H2O2	5.00E+12	0	17700	
1826	C6H12O1-5+HO2=>C2H4+CH2CH2COCH3+H2O2	5.00E+12	0	17700	
1827	C6H12O2-3+HO2=>CH3CHCO+NC3H7+H2O2	5.00E+12	0	17700	
1828	C6H12O2-4+HO2=>C3H6+C2H5CO+H2O2	5.00E+12	0	17700	
1829	C6H12O2-5+HO2=>CH3CHO+C4H71-3+H2O2	5.00E+12	0	17700	
1830	C6H12O3-4+HO2=>C2H5CHO+C3H5-S+H2O2	5.00E+12	0	17700	
1831	C6H12-1+OH=C6H12OH-1	1.00E+13	0	0	
1832	C6H12OH-1+O2=O2C6H12OH-1	6.00E+12	0	0	
1833	O2C6H12OH-1=NC4H9CHO+CH2O+OH	1.00E+12	0	27800	REV/1.0E12 0.0E0 -1.042E3/
1834	C6H12OH-2=C6H12-2+OH	1.07E+16	-1	29330	REV/2.0E12 0.0E0 0.0E0/
1835	O2C6H12OH-2=C6H12OH-2+O2	3.82E+21	-2.02	37830	
1836	O2C6H12OH-2=>NC3H7CHO+CH3CHO+OH	2.50E+10	0	18860	REV/1.0E12 0.0E0 -1.042E3/
1837	C6H12OH-3=C6H12-3+OH	3.90E+15	-0.93	29420	REV/2.0E12 0.0E0 0.0E0/
1838	O2C6H12OH-3=C6H12OH-3+O2	3.82E+21	-2.02	37830	
1839	O2C6H12OH-3=>OH+2C2H5CHO	2.50E+10	0	18860	REV/1.0E7 0.0E0 4.0E4/
1840	NC4H9CHO+O2=NC4H9CO+HO2	2.00E+13	0.5	42200	REV/2.143E10 7.3E-1 3.124E4/
1841	NC4H9CHO+OH=NC4H9CO+H2O	2.69E+10	0.76	-340	REV/1.8E13 0.0E0 2.4E4/
1842	NC4H9CHO+H=NC4H9CO+H2	4.00E+13	0	4200	REV/1.0E12 0.0E0 1.9E4/
1843	NC4H9CHO+O=NC4H9CO+OH	5.00E+12	0	1790	REV/1.0E12 0.0E0 1.0E4/
1844	NC4H9CHO+HO2=NC4H9CO+H2O2	2.80E+12	0	13600	REV/1.5E13 0.0E0 2.8E4/
1845	NC4H9CHO+CH3=NC4H9CO+CH4	1.70E+12	0	8440	REV/3.0E11 0.0E0 1.8E4/
1846	NC4H9CHO+CH3O=NC4H9CO+CH3OH	1.15E+11	0	1280	REV/2.5E10 0.0E0 1.0E4/
1847	NC4H9CHO+CH3O2=NC4H9CO+CH3O2H	1.00E+12	0	9500	REV/1.233E9 9.5E-1 2.104E4/
1848	NC4H9CHO+OH=C4H8CHO-1+H2O	5.27E+09	0.97	1586	REV/6.837E5 1.93E0 2.192E4/
1849	NC4H9CHO+OH=C4H8CHO-2+H2O	4.67E+07	1.61	-35	REV/6.837E5 1.93E0 2.192E4/
1850	NC4H9CHO+OH=C4H8CHO-3+H2O	4.67E+07	1.61	-35	REV/1.202E9 1.34E0 2.887E4/
1851	NC4H9CHO+OH=C4H8CHO-4+H2O	4.67E+07	1.61	-35	REV/1.0E11 0.0E0 0.0E0/
1852	NC4H9CO=PC4H9+CO	1.00E+11	0	9600	REV/2.5E11 0.0E0 7.8E3/
1853	C4H8CHO-1=C2H4+CH2CH2CHO	5.98E+18	-1.6	30430	REV/1.0E11 0.0E0 7.8E3/
1854	C4H8CHO-2=C3H6+CH2CHO	2.98E+14	-0.76	23320	REV/1.0E11 0.0E0 7.8E3/
1855	C4H8CHO-3=C4H8-1+HCO	4.80E+14	-0.72	24350	REV/1.0E11 0.0E0 7.8E3/

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Table B .1. (cont.)

1856	C4H8CHO-3=AC3H5CHO+CH3	3.64E+13	-0.36	30330	REV/1.0E11 0.0E0 7.8E3/
1857	C4H8CHO-4=C2H3CHO+C2H5	1.86E+18	-1.3	30830	REV/1.0E13 0.0E0 0.0E0/
1858	AC3H5CHO=C3H5-A+HCO	1.81E+19	-1.08	68480	REV/1.741E10 7.6E-1 3.12E4/
1859	AC3H5CHO+OH=AC3H5CO+H2O	2.69E+10	0.76	-340	REV/1.246E8 1.79E0 3.493E4/
1860	AC3H5CHO+OH=C2H3CHCHO+H2O	3.12E+06	2	-298	REV/1.152E13 -3.3E-1 1.199E4/
1861	AC3H5CHO+HO2=AC3H5CO+H2O2	3.00E+12	0	11920	REV/2.283E6 2.06E0 1.767E4/
1862	AC3H5CHO+HO2=C2H3CHCHO+H2O2	9.63E+03	2.6	13910	REV/1.579E13 -5.1E-1 1.127E4/
1863	AC3H5CHO+CH3O2=AC3H5CO+CH3O2H	1.00E+12	0	11920	REV/1.939E15 -7.2E-1 2.009E4/
1864	AC3H5CHO+CH3O2=C2H3CHCHO+CH3O2H	1.99E+12	0	17050	REV/1.5E11 0.0E0 4.81E3/
1865	AC3H5CO=C3H5-A+CO	6.20E+15	-1.09	-330	
1866	C2H3CHCHO+HO2=>C2H3CHO+HCO+OH	8.91E+12	0	0	REV/3.604E6 1.75E0 2.017E4/
1867	NC3H7COCH3+OH=C3H6COCH3-1+H2O	2.07E+07	1.73	753	REV/3.668E5 2.01E0 2.166E4/
1868	NC3H7COCH3+OH=C3H6COCH3-2+H2O	3.62E+07	1.64	-247	REV/2.368E13 -2.8E-1 2.87E4/
1869	NC3H7COCH3+OH=C3H6COCH3-3+H2O	8.45E+11	0	-228	REV/9.286E13 -7.4E-1 2.773E4/
1870	NC3H7COCH3+OH=NC3H7COCH2+H2O	5.10E+11	0	1192	REV/2.465E4 2.24E0 4.442E3/
1871	NC3H7COCH3+HO2=C3H6COCH3-1+H2O2	2.38E+04	2.55	16490	REV/3.373E11 5.0E-2 8.142E3/
1872	NC3H7COCH3+HO2=C3H6COCH3-2+H2O2	5.60E+12	0	17700	REV/3.327E13 -6.0E-1 6.16E3/
1873	NC3H7COCH3+HO2=C3H6COCH3-3+H2O2	2.00E+11	0	8698	REV/2.572E7 1.48E0 9.762E3/
1874	NC3H7COCH3+HO2=NC3H7COCH2+H2O2	2.38E+04	2.55	14690	REV/1.281E13 -4.9E-1 6.607E3/
1875	NC3H7COCH3+CH3O2=C3H6COCH3-1+CH3O2H	3.01E+12	0	19380	REV/4.926E11 -1.3E-1 6.774E3/
1876	NC3H7COCH3+CH3O2=C3H6COCH3-2+CH3O2H	1.99E+12	0	17050	REV/1.367E15 -7.8E-1 1.199E4/
1877	NC3H7COCH3+CH3O2=C3H6COCH3-3+CH3O2H	2.00E+12	0	15250	REV/1.337E16 -1.25E0 1.193E4/
1878	NC3H7COCH3+CH3O2=NC3H7COCH2+CH3O2H	3.01E+12	0	17580	REV/1.0E11 0.0E0 8.6E3/
1879	C3H6COCH3-1=C2H4+CH3COCH2	2.90E+16	-1.21	27000	REV/1.0E11 0.0E0 7.8E3/
1880	C3H6COCH3-2=C3H6+CH3CO	2.72E+16	-1.05	25590	REV/1.0E11 0.0E0 7.8E3/
1881	C3H6COCH3-3=C2H3COCH3+CH3	9.62E+15	-0.75	32390	REV/1.0E11 0.0E0 1.16E4/
1882	NC3H7COCH2=NC3H7+CH2CO	1.23E+18	-1.4	43450	REV/1.194E9 9.5E-1 2.103E4/
1883	C2H5COC2H5+OH=C2H5COC2H4P+H2O	1.05E+10	0.97	1586	REV/3.296E13 -3.2E-1 2.874E4/
1884	C2H5COC2H5+OH=C2H5COC2H4S+H2O	1.69E+12	0	-228	REV/3.201E4 2.2E0 4.472E3/
1885	C2H5COC2H5+HO2=C2H5COC2H4P+H2O2	4.76E+04	2.55	16490	REV/4.631E13 -6.5E-1 6.2E3/
1886	C2H5COC2H5+HO2=C2H5COC2H4S+H2O2	4.00E+11	0	8698	REV/1.949E10 3.1E-1 -1.882E3/
1887	C2H5COC2H5+O2=C2H5COC2H4P+HO2	4.10E+13	0	51310	REV/2.537E12 0.0E0 -1.702E3/
1888	C2H5COC2H5+O2=C2H5COC2H4S+HO2	3.10E+13	0	41970	REV/4.794E5 1.98E0 1.199E4/
1889	C2H5COC2H5+H=C2H5COC2H4P+H2	1.83E+07	2	7700	REV/4.036E7 1.68E0 1.701E4/
1890	C2H5COC2H5+H=C2H5COC2H4S+H2	8.96E+06	2	3200	REV/3.85E8 8.1E-1 1.404E4/
1891	C2H5COC2H5+C2H3=C2H5COC2H4P+C2H4	1.00E+12	0	10400	REV/3.976E10 5.0E-1 1.876E4/
1892	C2H5COC2H5+C2H3=C2H5COC2H4S+C2H4	6.00E+11	0	5600	REV/1.07E13 -5.8E-1 1.4E4/
1893	C2H5COC2H5+C2H5=C2H5COC2H4P+C2H6	1.00E+11	0	13400	REV/1.105E15 -8.9E-1 1.872E4/

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Table B .1. (cont.)

1894	C2H5COC2H5+C2H5=C2H5COC2H4S+C2H6	6.00E+10	0	8600	REV/5.475E9 0.0E0 9.02E3/
1895	C2H5COC2H5+CH3O=C2H5COC2H4P+CH3OH	4.34E+11	0	6460	REV/6.298E11 -3.0E-1 1.485E4/
1896	C2H5COC2H5+CH3O=C2H5COC2H4S+CH3OH	2.90E+11	0	2771	REV/1.664E13 -5.2E-1 6.642E3/
1897	C2H5COC2H5+CH3O2=C2H5COC2H4P+CH3O2H	6.02E+12	0	19380	REV/1.903E15 -8.3E-1 1.203E4/
1898	C2H5COC2H5+CH3O2=C2H5COC2H4S+CH3O2H	4.00E+12	0	15250	REV/8.0E10 0.0E0 1.13E4/
1899	C2H5COC2H4P=C2H5CO+C2H4	1.77E+17	-1.46	29540	REV/1.3E13 0.0E0 1.56E3/
1900	C2H5COC2H4S=C2H5COC2H3+H	8.70E+16	-0.82	42130	REV/1.673E11 -3.9E-1 1.822E4/
1901	C2H5COC2H3+OH=C2H5COCH2+CH2O	1.00E+10	0	0	REV/1.285E8 2.53E0 2.021E4/
1902	C2H5COC2H3+OH=PC2H4COC2H3+H2O	7.55E+09	0.97	1586	REV/1.35E13 -2.0E-1 2.86E4/
1903	C2H5COC2H3+OH=SC2H4COC2H3+H2O	8.45E+11	0	-228	REV/1.0E0 0.0E0 0.0E0/
1904	C2H5COC2H3+HO2=C2H5CO+CH2CHO+OH	6.03E+09	0	7949	REV/2.405E3 3.78E0 3.652E3/
1905	C2H5COC2H3+HO2=PC2H4COC2H3+H2O2	2.38E+04	2.55	16490	REV/1.896E13 -5.3E-1 6.065E3/
1906	C2H5COC2H3+HO2=SC2H4COC2H3+H2O2	2.00E+11	0	8698	REV/1.0E0 0.0E0 0.0E0/
1907	C2H5COC2H3+CH3O2=C2H5CO+CH2CHO+CH3O	3.97E+11	0	17050	REV/1.25E12 1.06E0 5.822E3/
1908	C2H5COC2H3+CH3O2=PC2H4COC2H3+CH3O2H	3.01E+12	0	19380	REV/7.793E14 -7.1E-1 1.19E4/
1909	C2H5COC2H3+CH3O2=SC2H4COC2H3+CH3O2H	2.00E+12	0	15250	REV/8.0E10 0.0E0 1.13E4/
1910	PC2H4COC2H3=C2H3CO+C2H4	5.26E+14	0.38	21460	REV/8.0E10 0.0E0 1.26E4/
1911	SC2H4COC2H3=CH3CHCO+C2H3	1.64E+16	-0.74	54590	REV/7.264E84 -2.081E1 4.156E4/
1912	NC7H16=H+C7H15-1	2.68E+88	-21.17	142800	REV/2.263E83 -2.031E1 4.083E4/
1913	NC7H16=H+C7H15-2	1.30E+88	-21.01	139500	REV/2.263E83 -2.031E1 4.083E4/
1914	NC7H16=H+C7H15-3	1.30E+88	-21.01	139500	REV/2.255E83 -2.031E1 4.083E4/
1915	NC7H16=H+C7H15-4	6.50E+87	-21.01	139500	LOW/4.963E42 -7.78E0 4.28E4/ TROE/8.92E-1 1.0E10 2.228E0 1.798E9/
1916	NC7H16(+M)=C6H13-1+CH3(+M)	4.33E+24	-2.12	89900	LOW/3.753E48 -9.46E0 4.131E4/ TROE/9.0E-2 3.6556E0 1.0E10 9.33E9/
1917	NC7H16(+M)=C5H11-1+C2H5(+M)	6.82E+26	-2.7	88910	LOW/6.509E48 -9.57E0 4.129E4/ TROE/9.11E-1 1.0E10 2.2382E1 5.0E9/
1918	NC7H16(+M)=PC4H9+NC3H7(+M)	1.36E+26	-2.53	88760	REV/2.037E1 3.38E0 8.618E3/
1919	NC7H16+H=C7H15-1+H2	1.88E+05	2.75	6280	REV/1.807E1 3.38E0 9.318E3/
1920	NC7H16+H=C7H15-2+H2	2.60E+06	2.4	4471	REV/1.807E1 3.38E0 9.318E3/
1921	NC7H16+H=C7H15-3+H2	2.60E+06	2.4	4471	REV/1.8E1 3.38E0 9.318E3/
1922	NC7H16+H=C7H15-4+H2	1.30E+06	2.4	4471	REV/1.085E1 3.29E0 4.642E3/
1923	NC7H16+O=C7H15-1+OH	1.93E+05	2.68	3716	REV/3.481E-1 3.67E0 5.541E3/
1924	NC7H16+O=C7H15-2+OH	9.54E+04	2.71	2106	REV/3.481E-1 3.67E0 5.541E3/
1925	NC7H16+O=C7H15-3+OH	9.54E+04	2.71	2106	REV/3.468E-1 3.67E0 5.541E3/
1926	NC7H16+O=C7H15-4+OH	4.77E+04	2.71	2106	REV/2.952E4 2.33E0 1.818E4/
1927	NC7H16+OH=C7H15-1+H2O	2.57E+07	1.8	954	REV/3.624E2 2.87E0 1.914E4/
1928	NC7H16+OH=C7H15-2+H2O	4.90E+06	2	-596	REV/3.624E2 2.87E0 1.914E4/
1929	NC7H16+OH=C7H15-3+H2O	4.90E+06	2	-596	REV/3.61E2 2.87E0 1.914E4/

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Table B .1. (cont.)

1930	NC7H16+OH=C7H15-4+H2O	2.45E+06	2	-596	REV/2.557E0 3.53E0 3.498E3/
1931	NC7H16+HO2=C7H15-1+H2O2	4.08E+01	3.59	17160	REV/4.982E-1 3.66E0 2.562E3/
1932	NC7H16+HO2=C7H15-2+H2O2	1.26E+02	3.37	13720	REV/4.982E-1 3.66E0 2.562E3/
1933	NC7H16+HO2=C7H15-3+H2O2	1.26E+02	3.37	13720	REV/4.952E-1 3.66E0 2.562E3/
1934	NC7H16+HO2=C7H15-4+H2O2	6.32E+01	3.37	13720	REV/8.935E-2 3.84E0 1.103E4/
1935	NC7H16+CH3=C7H15-1+CH4	9.04E-01	3.65	7154	REV/3.432E2 2.79E0 1.367E4/
1936	NC7H16+CH3=C7H15-2+CH4	5.41E+04	2.26	7287	REV/3.432E2 2.79E0 1.367E4/
1937	NC7H16+CH3=C7H15-3+CH4	5.41E+04	2.26	7287	REV/3.419E2 2.79E0 1.367E4/
1938	NC7H16+CH3=C7H15-4+CH4	2.71E+04	2.26	7287	REV/2.386E10 2.8E-1 4.53E2/
1939	NC7H16+O2=C7H15-1+HO2	4.20E+13	0	52800	REV/1.0E9 6.3E-1 3.09E2/
1940	NC7H16+O2=C7H15-2+HO2	2.80E+13	0	50150	REV/1.0E9 6.3E-1 3.09E2/
1941	NC7H16+O2=C7H15-3+HO2	2.80E+13	0	50150	REV/9.941E8 6.3E-1 3.09E2/
1942	NC7H16+O2=C7H15-4+HO2	1.40E+13	0	50150	REV/3.2E11 0.0E0 1.23E4/
1943	NC7H16+C2H5=C7H15-1+C2H6	1.00E+11	0	13400	REV/1.0E11 0.0E0 1.29E4/
1944	NC7H16+C2H5=C7H15-2+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
1945	NC7H16+C2H5=C7H15-3+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
1946	NC7H16+C2H5=C7H15-4+C2H6	5.00E+10	0	10400	REV/1.2E10 0.0E0 9.2E3/
1947	NC7H16+CH3O=C7H15-1+CH3OH	3.16E+11	0	7000	REV/8.9E9 0.0E0 7.2E3/
1948	NC7H16+CH3O=C7H15-2+CH3OH	2.19E+11	0	5000	REV/8.9E9 0.0E0 7.2E3/
1949	NC7H16+CH3O=C7H15-3+CH3OH	2.19E+11	0	5000	REV/8.9E9 0.0E0 7.2E3/
1950	NC7H16+CH3O=C7H15-4+CH3OH	1.10E+11	0	5000	REV/2.57E12 0.0E0 2.54E4/
1951	NC7H16+C2H3=C7H15-1+C2H4	1.00E+12	0	18000	REV/2.0E12 0.0E0 2.42E4/
1952	NC7H16+C2H3=C7H15-2+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
1953	NC7H16+C2H3=C7H15-3+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
1954	NC7H16+C2H3=C7H15-4+C2H4	4.00E+11	0	16800	REV/1.69E0 3.46E0 3.024E3/
1955	NC7H16+CH3O2=C7H15-1+CH3O2H	1.39E+00	3.97	18280	REV/1.562E0 3.42E0 2.054E3/
1956	NC7H16+CH3O2=C7H15-2+CH3O2H	2.04E+01	3.58	14810	REV/1.562E0 3.42E0 2.054E3/
1957	NC7H16+CH3O2=C7H15-3+CH3O2H	2.04E+01	3.58	14810	REV/1.553E0 3.42E0 2.054E3/
1958	NC7H16+CH3O2=C7H15-4+CH3O2H	1.02E+01	3.58	14810	REV/1.17E3 2.25E0 3.057E3/
1959	NC7H16+O2CHO=C7H15-1+HO2CHO	1.68E+13	0	20440	REV/2.482E1 2.64E0 2.823E3/
1960	NC7H16+O2CHO=C7H15-2+HO2CHO	1.12E+13	0	17690	REV/2.482E1 2.64E0 2.823E3/
1961	NC7H16+O2CHO=C7H15-3+HO2CHO	1.12E+13	0	17690	REV/2.472E1 2.64E0 2.823E3/
1962	NC7H16+O2CHO=C7H15-4+HO2CHO	5.60E+12	0	17690	REV/1.44E10 0.0E0 1.5E4/
1963	NC7H16+C7H15O2-1=C7H15-1+C7H15O2H-1	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1964	NC7H16+C7H15O2-2=C7H15-1+C7H15O2H-2	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1965	NC7H16+C7H15O2-3=C7H15-1+C7H15O2H-3	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1966	NC7H16+C7H15O2-4=C7H15-1+C7H15O2H-4	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
1967	NC7H16+C7H15O2-1=C7H15-2+C7H15O2H-1	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1968	NC7H16+C7H15O2-2=C7H15-2+C7H15O2H-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1969	NC7H16+C7H15O2-3=C7H15-2+C7H15O2H-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1970	NC7H16+C7H15O2-4=C7H15-2+C7H15O2H-4	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1971	NC7H16+C7H15O2-1=C7H15-3+C7H15O2H-1	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/

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Table B .1. (cont.)

1972	NC7H16+C7H15O2-2=C7H15-3+C7H15O2H-2	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1973	NC7H16+C7H15O2-3=C7H15-3+C7H15O2H-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1974	NC7H16+C7H15O2-4=C7H15-3+C7H15O2H-4	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1975	NC7H16+C7H15O2-1=C7H15-4+C7H15O2H-1	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1976	NC7H16+C7H15O2-2=C7H15-4+C7H15O2H-2	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1977	NC7H16+C7H15O2-3=C7H15-4+C7H15O2H-3	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
1978	NC7H16+C7H15O2-4=C7H15-4+C7H15O2H-4	4.03E+12	0	17700	REV/1.5E11 0.0E0 1.23E4/
1979	NC7H16+C7H15-1=C7H15-2+NC7H16	1.00E+11	0	10400	REV/1.5E11 0.0E0 1.23E4/
1980	NC7H16+C7H15-1=C7H15-3+NC7H16	1.00E+11	0	10400	REV/1.5E11 0.0E0 1.23E4/
1981	NC7H16+C7H15-1=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.04E4/
1982	NC7H16+C7H15-2=C7H15-3+NC7H16	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.04E4/
1983	NC7H16+C7H15-2=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.04E4/
1984	NC7H16+C7H15-3=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.0E11 0.0E0 8.2E3/
1985	C7H15-1=C5H11-1+C2H4	1.23E+19	-1.91	31400	REV/1.0E13 0.0E0 2.9E3/
1986	C7H15-1=C7H14-1+H	9.65E+13	-0.26	36010	REV/1.0E11 0.0E0 8.2E3/
1987	C7H15-2=PC4H9+C3H6	9.76E+18	-1.79	31360	REV/1.0E13 0.0E0 1.2E3/
1988	C7H15-2=C7H14-1+H	6.07E+12	0.09	36810	REV/1.0E13 0.0E0 2.9E3/
1989	C7H15-2=C7H14-2+H	1.23E+13	-0.08	35640	REV/1.0E11 0.0E0 7.7E3/
1990	C7H15-3=C4H8-1+NC3H7	6.17E+18	-1.71	30960	REV/1.75E11 0.0E0 7.2E3/
1991	C7H15-3=C6H12-1+CH3	2.70E+17	-1.35	31480	REV/1.0E13 0.0E0 2.9E3/
1992	C7H15-3=C7H14-2+H	1.23E+13	-0.08	35640	REV/1.0E13 0.0E0 2.9E3/
1993	C7H15-3=C7H14-3+H	9.15E+12	-0.02	35730	REV/1.0E11 0.0E0 8.2E3/
1994	C7H15-4=C2H5+C5H10-1	1.14E+18	-1.34	31430	REV/1.0E13 0.0E0 2.9E3/
1995	C7H15-4=C7H14-3+H	1.82E+13	-0.02	35730	REV/6.517E-10 1.8E-1 1.876E4/
1996	C7H15-1+O2=C7H14-1+HO2	3.00E-09	0	3000	REV/1.532E-8 -1.6E-1 1.827E4/
1997	C7H15-2+O2=C7H14-1+HO2	4.50E-09	0	5020	REV/5.04E-9 1.0E-2 1.912E4/
1998	C7H15-2+O2=C7H14-2+HO2	3.00E-09	0	3000	REV/5.04E-9 1.0E-2 1.912E4/
1999	C7H15-3+O2=C7H14-2+HO2	3.00E-09	0	3000	REV/6.769E-9 -5.0E-2 1.903E4/
2000	C7H15-3+O2=C7H14-3+HO2	3.00E-09	0	3000	REV/6.795E-9 -5.0E-2 1.903E4/
2001	C7H15-4+O2=C7H14-3+HO2	6.00E-09	0	3000	REV/8.716E7 1.33E0 3.627E4/
2002	C7H15-1=C7H15-3	1.39E+09	0.98	33760	REV/3.176E8 7.0E-1 2.227E4/
2003	C7H15-1=C7H15-4	2.54E+09	0.35	19760	REV/9.587E8 1.39E0 3.97E4/
2004	C7H15-2=C7H15-3	9.59E+08	1.39	39700	REV/3.445E7 1.97E0 4.127E4/
2005	C7H15-1=C7H15-2	5.48E+08	1.62	38760	REV/4.393E6 2.1E0 2.062E4/
2006	C7H14-1+H=C7H131-3+H2	3.38E+05	2.36	207	REV/3.834E3 2.74E0 1.154E4/
2007	C7H14-1+H=C7H131-4+H2	1.30E+06	2.4	4471	REV/3.834E3 2.74E0 1.154E4/
2008	C7H14-1+H=C7H131-5+H2	1.30E+06	2.4	4471	REV/3.834E3 2.74E0 1.154E4/
2009	C7H14-1+H=C7H131-6+H2	1.30E+06	2.4	4471	REV/3.056E4 2.54E0 1.132E4/
2010	C7H14-1+H=C7H131-7+H2	6.65E+05	2.54	6756	REV/1.557E6 2.38E0 3.365E4/
2011	C7H14-1+OH=C7H131-3+H2O	2.76E+04	2.64	-1919	REV/5.963E5 1.95E0 2.219E4/
2012	C7H14-1+OH=C7H131-4+H2O	4.67E+07	1.61	-35	REV/5.963E5 1.95E0 2.219E4/

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Table B .1. (cont.)

2013	C7H14-1+OH=C7H131-5+H2O	4.67E+07	1.61	-35	REV/5.963E5 1.95E0 2.219E4/
2014	C7H14-1+OH=C7H131-6+H2O	4.67E+07	1.61	-35	REV/1.049E9 9.7E-1 2.13E4/
2015	C7H14-1+OH=C7H131-7+H2O	5.27E+09	0.97	1586	REV/1.254E3 3.05E0 2.489E4/
2016	C7H14-1+CH3=C7H131-3+CH4	3.69E+00	3.31	4002	REV/1.163E-1 3.8E0 1.303E4/
2017	C7H14-1+CH3=C7H131-4+CH4	1.51E+00	3.46	5481	REV/1.163E-1 3.8E0 1.303E4/
2018	C7H14-1+CH3=C7H131-5+CH4	1.51E+00	3.46	5481	REV/1.163E-1 3.8E0 1.303E4/
2019	C7H14-1+CH3=C7H131-6+CH4	1.51E+00	3.46	5481	REV/5.427E-1 3.65E0 1.219E4/
2020	C7H14-1+CH3=C7H131-7+CH4	4.52E-01	3.65	7154	REV/1.612E6 1.96E0 1.463E4/
2021	C7H14-1+HO2=C7H131-3+H2O2	4.82E+03	2.55	10530	REV/7.307E2 2.62E0 4.672E3/
2022	C7H14-1+HO2=C7H131-4+H2O2	9.64E+03	2.6	13910	REV/7.307E2 2.62E0 4.672E3/
2023	C7H14-1+HO2=C7H131-5+H2O2	9.64E+03	2.6	13910	REV/7.307E2 2.62E0 4.672E3/
2024	C7H14-1+HO2=C7H131-6+H2O2	9.64E+03	2.6	13910	REV/2.811E4 2.22E0 4.746E3/
2025	C7H14-1+HO2=C7H131-7+H2O2	2.38E+04	2.55	16490	REV/3.357E6 1.79E0 1.161E4/
2026	C7H14-1+CH3O2=C7H131-3+CH3O2H	4.82E+03	2.55	10530	REV/1.521E3 2.44E0 1.652E3/
2027	C7H14-1+CH3O2=C7H131-4+CH3O2H	9.64E+03	2.6	13910	REV/1.521E3 2.44E0 1.652E3/
2028	C7H14-1+CH3O2=C7H131-5+CH3O2H	9.64E+03	2.6	13910	REV/1.521E3 2.44E0 1.652E3/
2029	C7H14-1+CH3O2=C7H131-6+CH3O2H	9.64E+03	2.6	13910	REV/5.853E4 2.04E0 1.726E3/
2030	C7H14-1+CH3O2=C7H131-7+CH3O2H	2.38E+04	2.55	16490	REV/2.51E2 2.66E0 2.729E4/
2031	C7H14-1+CH3O=C7H131-3+CH3OH	4.00E+01	2.9	8609	REV/2.062E8 3.7E-1 9.911E3/
2032	C7H14-1+CH3O=C7H131-4+CH3OH	1.45E+11	0	4571	REV/2.062E8 3.7E-1 9.911E3/
2033	C7H14-1+CH3O=C7H131-5+CH3OH	1.45E+11	0	4571	REV/2.062E8 3.7E-1 9.911E3/
2034	C7H14-1+CH3O=C7H131-6+CH3OH	1.45E+11	0	4571	REV/4.808E9 2.0E-2 9.288E3/
2035	C7H14-1+CH3O=C7H131-7+CH3OH	2.17E+11	0	6458	REV/4.561E6 2.06E0 2.003E4/
2036	C7H14-2+H=C7H131-3+H2	1.73E+05	2.5	2492	REV/4.4E6 2.1E0 2.059E4/
2037	C7H14-2+H=C7H132-4+H2	3.38E+05	2.36	207	REV/3.843E3 2.74E0 1.152E4/
2038	C7H14-2+H=C7H132-5+H2	1.30E+06	2.4	4471	REV/3.843E3 2.74E0 1.152E4/
2039	C7H14-2+H=C7H132-6+H2	1.30E+06	2.4	4471	REV/3.149E4 2.53E0 1.13E4/
2040	C7H14-2+H=C7H132-7+H2	6.65E+05	2.54	6756	REV/3.561E8 1.56E0 3.24E4/
2041	C7H14-2+OH=C7H131-3+H2O	3.12E+06	2	-298	REV/1.56E6 2.38E0 3.362E4/
2042	C7H14-2+OH=C7H132-4+H2O	2.76E+04	2.64	-1919	REV/5.978E3 1.95E0 2.217E4/
2043	C7H14-2+OH=C7H132-5+H2O	4.67E+05	1.61	-35	REV/5.978E3 1.95E0 2.217E4/
2044	C7H14-2+OH=C7H132-6+H2O	4.67E+05	1.61	-35	REV/1.08E9 9.6E-1 2.128E4/
2045	C7H14-2+OH=C7H132-7+H2O	5.27E+09	0.97	1586	REV/1.522E3 3.06E0 2.37E4/
2046	C7H14-2+CH3=C7H131-3+CH4	2.21E+00	3.5	5675	REV/1.256E3 3.05E0 2.486E4/
2047	C7H14-2+CH3=C7H132-4+CH4	3.69E+00	3.31	4002	REV/1.166E-1 3.8E0 1.301E4/
2048	C7H14-2+CH3=C7H132-5+CH4	1.51E+00	3.46	5481	REV/1.166E-1 3.8E0 1.301E4/

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Table B .1. (cont.)

2049	C7H14-2+CH3=C7H132-6+CH4	1.51E+00	3.46	5481	REV/5.591E-1 3.64E0 1.217E4/
2050	C7H14-2+CH3=C7H132-7+CH4	4.52E-01	3.65	7154	REV/6.531E6 1.84E0 1.514E4/
2051	C7H14-2+HO2=C7H131-3+H2O2	9.64E+03	2.6	13910	REV/1.615E6 1.96E0 1.46E4/
2052	C7H14-2+HO2=C7H132-4+H2O2	4.82E+03	2.55	10530	REV/7.325E2 2.62E0 4.652E3/
2053	C7H14-2+HO2=C7H132-5+H2O2	9.64E+03	2.6	13910	REV/7.325E2 2.62E0 4.652E3/
2054	C7H14-2+HO2=C7H132-6+H2O2	9.64E+03	2.6	13910	REV/2.896E4 2.21E0 4.726E3/
2055	C7H14-2+HO2=C7H132-7+H2O2	2.38E+04	2.55	16490	REV/1.36E7 1.66E0 1.212E4/
2056	C7H14-2+CH3O2=C7H131-3+CH3O2H	9.64E+03	2.6	13910	REV/3.362E6 1.79E0 1.158E4/
2057	C7H14-2+CH3O2=C7H132-4+CH3O2H	4.82E+03	2.55	10530	REV/1.525E3 2.44E0 1.632E3/
2058	C7H14-2+CH3O2=C7H132-5+CH3O2H	9.64E+03	2.6	13910	REV/1.525E3 2.44E0 1.632E3/
2059	C7H14-2+CH3O2=C7H132-6+CH3O2H	9.64E+03	2.6	13910	REV/6.03E4 2.04E0 1.706E3/
2060	C7H14-2+CH3O2=C7H132-7+CH3O2H	2.38E+04	2.55	16490	REV/1.144E3 2.54E0 2.78E4/
2061	C7H14-2+CH3O=C7H131-3+CH3OH	9.00E+01	2.95	11990	REV/2.513E2 2.66E0 2.726E4/
2062	C7H14-2+CH3O=C7H132-4+CH3OH	4.00E+01	2.9	8609	REV/2.067E8 3.7E-1 9.891E3/
2063	C7H14-2+CH3O=C7H132-5+CH3OH	1.45E+11	0	4571	REV/2.067E8 3.7E-1 9.891E3/
2064	C7H14-2+CH3O=C7H132-6+CH3OH	1.45E+11	0	4571	REV/4.953E9 2.0E-2 9.268E3/
2065	C7H14-2+CH3O=C7H132-7+CH3OH	2.17E+11	0	6458	REV/3.097E4 2.53E0 1.126E4/
2066	C7H14-3+H=C7H133-1+H2	6.65E+05	2.54	6756	REV/3.276E6 2.16E0 2.068E4/
2067	C7H14-3+H=C7H132-4+H2	3.38E+05	2.36	207	REV/4.38E6 2.1E0 2.056E4/
2068	C7H14-3+H=C7H133-5+H2	3.38E+05	2.36	207	REV/3.916E3 2.74E0 1.149E4/
2069	C7H14-3+H=C7H133-6+H2	1.30E+06	2.4	4471	REV/3.097E4 2.53E0 1.126E4/
2070	C7H14-3+H=C7H133-7+H2	6.65E+05	2.54	6756	REV/2.125E9 9.6E-1 2.124E4/
2071	C7H14-3+OH=C7H133-1+H2O	1.05E+10	0.97	1586	REV/1.161E6 2.44E0 3.371E4/
2072	C7H14-3+OH=C7H132-4+H2O	2.76E+04	2.64	-1919	REV/1.552E6 2.38E0 3.359E4/
2073	C7H14-3+OH=C7H133-5+H2O	2.76E+04	2.64	-1919	REV/6.091E5 1.95E0 2.214E4/
2074	C7H14-3+OH=C7H133-6+H2O	4.67E+07	1.61	-35	REV/2.125E9 9.6E-1 2.124E4/
2075	C7H14-3+OH=C7H133-7+H2O	1.05E+10	0.97	1586	REV/1.1E0 3.64E0 1.213E4/
2076	C7H14-3+CH3=C7H133-1+CH4	9.04E-01	3.65	7154	REV/9.355E2 3.11E0 2.495E4/
2077	C7H14-3+CH3=C7H132-4+CH4	3.69E+00	3.31	4002	REV/1.251E3 3.05E0 2.483E4/
2078	C7H14-3+CH3=C7H133-5+CH4	3.69E+00	3.31	4002	REV/1.188E-1 3.8E0 1.298E4/
2079	C7H14-3+CH3=C7H133-6+CH4	1.51E+00	3.46	5481	REV/1.1E0 3.64E0 1.213E4/
2080	C7H14-3+CH3=C7H133-7+CH4	9.04E-01	3.65	7154	REV/5.697E4 2.22E0 4.686E3/
2081	C7H14-3+HO2=C7H133-1+H2O2	4.76E+04	2.55	16490	REV/1.202E6 2.03E0 1.469E4/
2082	C7H14-3+HO2=C7H132-4+H2O2	4.82E+03	2.55	10530	REV/1.607E6 1.96E0 1.457E4/
2083	C7H14-3+HO2=C7H133-5+H2O2	4.82E+03	2.55	10530	REV/7.464E2 2.61E0 4.622E3/
2084	C7H14-3+HO2=C7H133-6+H2O2	9.64E+03	2.6	13910	REV/5.697E4 2.22E0 4.686E3/

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Table B .1. (cont.)

2085	C7H14-3+HO2=C7H133-7+H2O2	4.76E+04	2.55	16490	REV/1.186E5 2.04E0 1.666E3/
2086	C7H14-3+CH3O2=C7H133-1+CH3O2H	4.76E+04	2.55	16490	REV/2.503E6 1.85E0 1.167E4/
2087	C7H14-3+CH3O2=C7H132-4+CH3O2H	4.82E+03	2.55	10530	REV/3.346E6 1.79E0 1.155E4/
2088	C7H14-3+CH3O2=C7H133-5+CH3O2H	4.82E+03	2.55	10530	REV/1.554E3 2.44E0 1.602E3/
2089	C7H14-3+CH3O2=C7H133-6+CH3O2H	9.64E+03	2.6	13910	REV/1.186E5 2.04E0 1.666E3/
2090	C7H14-3+CH3O2=C7H133-7+CH3O2H	4.76E+04	2.55	16490	REV/9.743E9 2.0E-2 9.228E3/
2091	C7H14-3+CH3O=C7H133-1+CH3OH	4.34E+11	0	6458	REV/1.871E2 2.73E0 2.735E4/
2092	C7H14-3+CH3O=C7H132-4+CH3OH	4.00E+01	2.9	8609	REV/2.502E2 2.66E0 2.723E4/
2093	C7H14-3+CH3O=C7H133-5+CH3OH	4.00E+01	2.9	8609	REV/2.106E8 3.7E-1 9.861E3/
2094	C7H14-3+CH3O=C7H133-6+CH3OH	1.45E+11	0	4571	REV/9.743E9 2.0E-2 9.228E3/
2095	C7H14-3+CH3O=C7H133-7+CH3OH	4.34E+11	0	6458	REV/4.435E15 -1.02E0 1.54E4/
2096	C7H131-3+HO2=C7H13O1-3+OH	9.64E+12	0	0	REV/4.332E17 -1.6E0 2.016E4/
2097	C7H131-3+CH3O2=C7H13O1-3+CH3O	9.64E+12	0	0	REV/2.836E14 -6.8E-1 1.8E4/
2098	C7H131-3+C2H5O2=C7H13O1-3+C2H5O	9.64E+12	0	0	REV/8.5E10 0.0E0 8.3E3/
2099	C7H131-3=C4H6+NC3H7	1.11E+19	-1.53	40700	REV/8.5E10 0.0E0 8.3E3/
2100	C7H131-4=C5H10-1+C2H3	2.49E+12	0.03	37300	REV/8.5E10 0.0E0 8.3E3/
2101	C7H131-4=C5H81-3+C2H5	2.29E+14	-0.68	22050	REV/5.0E10 0.0E0 8.3E3/
2102	C7H131-5=C4H8-1+C3H5-A	6.18E+15	-1.18	17980	REV/1.0E11 0.0E0 8.3E3/
2103	C7H131-6=C3H6+C4H71-4	1.24E+17	-1.17	30740	REV/1.0E11 0.0E0 8.3E3/
2104	C7H131-7=C2H4+C5H91-5	9.42E+17	-1.56	31180	REV/4.273E15 -1.02E0 1.543E4/
2105	C7H132-4+HO2=C7H13O2-4+OH	9.64E+12	0	0	REV/4.173E17 -1.59E0 2.019E4/
2106	C7H132-4+CH3O2=C7H13O2-4+CH3O	9.64E+12	0	0	REV/2.732E14 -6.7E-1 1.803E4/
2107	C7H132-4+C2H5O2=C7H13O2-4+C2H5O	9.64E+12	0	0	REV/1.0E11 0.0E0 8.3E3/
2108	C7H132-5=C4H8-1+C3H5-S	9.42E+17	-1.49	44260	REV/1.0E11 0.0E0 8.3E3/
2109	C7H132-6=C3H6+C4H71-3	2.19E+14	-0.74	17740	REV/1.0E11 0.0E0 8.3E3/
2110	C7H132-7=C2H4+C5H92-5	9.79E+17	-1.57	31160	REV/1.0E11 0.0E0 8.3E3/
2111	C7H133-1=C2H4+C5H91-1	1.01E+17	-1.32	43990	REV/1.182E15 -8.4E-1 1.527E4/
2112	C7H133-5+HO2=C7H13O3-5+OH	9.64E+12	0	0	REV/1.155E17 -1.42E0 2.003E4/
2113	C7H133-5+CH3O2=C7H13O3-5+CH3O	9.64E+12	0	0	REV/7.559E13 -5.0E-1 1.787E4/
2114	C7H133-5+C2H5O2=C7H13O3-5+C2H5O	9.64E+12	0	0	REV/1.0E11 0.0E0 8.3E3/
2115	C7H133-6=C3H6+C4H71-1	1.35E+16	-0.92	43560	REV/1.0E11 0.0E0 8.3E3/
2116	C7H133-7=C2H4+C5H91-3	2.27E+15	-1.2	18050	REV/1.0E11 0.0E0 9.6E3/
2117	C7H13O1-3=C2H3CHO+PC4H9	9.63E+19	-1.96	10850	REV/1.0E11 0.0E0 9.6E3/
2118	C7H13O1-3=NC4H9CHO+C2H3	1.03E+18	-1.51	23300	REV/1.0E11 0.0E0 9.6E3/
2119	C7H13O2-4=SC3H5CHO+NC3H7	6.32E+19	-1.93	11130	REV/1.0E11 0.0E0 9.6E3/
2120	C7H13O2-4=NC3H7CHO+C3H5-S	1.01E+22	-2.46	29190	REV/1.0E11 0.0E0 9.6E3/
2121	C7H13O3-5=C4H7CHO1-1+C2H5	6.03E+18	-1.62	10450	REV/1.0E11 0.0E0 9.6E3/
2122	C7H13O3-5=C2H5CHO+C4H71-1	6.43E+21	-2.43	30090	
2123	C7H14-1+OH=>CH2O+C6H13-1	1.00E+11	0	-4000	
2124	C7H14-1+OH=>CH3CHO+C5H11-1	1.00E+11	0	-4000	
2125	C7H14-2+OH=>CH3CHO+C5H11-1	1.00E+11	0	-4000	

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Table B .1. (cont.)

2126	C7H14-2+OH=>C2H5CHO+PC4H9	1.00E+11	0	-4000	
2127	C7H14-3+OH=>C2H5CHO+PC4H9	1.00E+11	0	-4000	
2128	C7H14-1+O=>CH2CHO+C5H11-1	1.00E+11	0	-1050	
2129	C7H14-2+O=>CH3CHO+C5H10-1	1.00E+11	0	-1050	
2130	C7H14-3+O=>CH3CHO+C5H10-1	1.00E+11	0	-1050	REV/1.0E13 0.0E0 0.0E0/
2131	C7H14-1=PC4H9+C3H5-A	3.17E+21	-1.62	75330	REV/1.0E13 0.0E0 0.0E0/
2132	C7H14-2=C4H71-3+NC3H7	3.74E+21	-1.74	75710	REV/1.0E13 0.0E0 0.0E0/
2133	C7H14-3=C5H91-3+C2H5	5.95E+21	-1.85	75790	REV/4.52E12 0.0E0 0.0E0/
2134	C7H15O2-1=C7H15-1+O2	2.66E+20	-1.67	35400	REV/7.54E12 0.0E0 0.0E0/
2135	C7H15O2-2=C7H15-2+O2	1.36E+23	-2.36	37670	REV/7.54E12 0.0E0 0.0E0/
2136	C7H15O2-3=C7H15-3+O2	1.36E+23	-2.36	37670	REV/7.54E12 0.0E0 0.0E0/
2137	C7H15O2-4=C7H15-4+O2	1.36E+23	-2.36	37670	REV/1.116E14 -2.3E-1 3.025E4/
2138	C7H15-1+C7H15O2-1=2C7H15O-1	7.00E+12	0	-1000	REV/6.348E13 -1.6E-1 2.988E4/
2139	C7H15-1+C7H15O2-2=C7H15O-1+C7H15O-2	7.00E+12	0	-1000	REV/6.348E13 -1.6E-1 2.988E4/
2140	C7H15-1+C7H15O2-3=C7H15O-1+C7H15O-3	7.00E+12	0	-1000	REV/6.348E13 -1.6E-1 2.988E4/
2141	C7H15-1+C7H15O2-4=C7H15O-1+C7H15O-4	7.00E+12	0	-1000	REV/9.689E15 -8.0E-1 3.216E4/
2142	C7H15-2+C7H15O2-1=C7H15O-2+C7H15O-1	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2143	C7H15-2+C7H15O2-2=2C7H15O-2	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2144	C7H15-2+C7H15O2-3=C7H15O-2+C7H15O-3	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2145	C7H15-2+C7H15O2-4=C7H15O-2+C7H15O-4	7.00E+12	0	-1000	REV/9.689E15 -8.0E-1 3.216E4/
2146	C7H15-3+C7H15O2-1=C7H15O-3+C7H15O-1	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2147	C7H15-3+C7H15O2-2=C7H15O-3+C7H15O-2	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2148	C7H15-3+C7H15O2-3=2C7H15O-3	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2149	C7H15-3+C7H15O2-4=C7H15O-3+C7H15O-4	7.00E+12	0	-1000	REV/9.689E15 -8.0E-1 3.216E4/
2150	C7H15-4+C7H15O2-1=C7H15O-4+C7H15O-1	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2151	C7H15-4+C7H15O2-2=C7H15O-4+C7H15O-2	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
2152	C7H15-4+C7H15O2-3=C7H15O-4+C7H15O-3	7.00E+12	0	-1000	REV/5.511E15 -7.3E-1 3.179E4/
2153	C7H15-4+C7H15O2-4=2C7H15O-4	7.00E+12	0	-1000	REV/3.549E15 -5.7E-1 2.616E4/
2154	C7H15-1+HO2=C7H15O-1+OH	7.00E+12	0	-1000	REV/3.081E17 -1.15E0 2.807E4/
2155	C7H15-2+HO2=C7H15O-2+OH	7.00E+12	0	-1000	REV/3.081E17 -1.15E0 2.807E4/
2156	C7H15-3+HO2=C7H15O-3+OH	7.00E+12	0	-1000	REV/3.081E17 -1.15E0 2.807E4/
2157	C7H15-4+HO2=C7H15O-4+OH	7.00E+12	0	-1000	REV/2.22E14 -2.8E-1 3.04E4/
2158	C7H15-1+CH3O2=C7H15O-1+CH3O	7.00E+12	0	-1000	REV/1.927E16 -8.5E-1 3.231E4/
2159	C7H15-2+CH3O2=C7H15O-2+CH3O	7.00E+12	0	-1000	REV/1.927E16 -8.5E-1 3.231E4/
2160	C7H15-3+CH3O2=C7H15O-3+CH3O	7.00E+12	0	-1000	REV/1.927E16 -8.5E-1 3.231E4/
2161	C7H15-4+CH3O2=C7H15O-4+CH3O	7.00E+12	0	-1000	
2162	C7H15O2-1=C7H14-1+HO2	1.00E+39	-8.11	41490	
2163	C7H15O2-2=C7H14-1+HO2	1.01E+43	-9.41	42490	
2164	C7H15O2-2=C7H14-2+HO2	1.00E+39	-8.11	41490	
2165	C7H15O2-3=C7H14-2+HO2	1.00E+39	-8.11	41490	

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Table B .1. (cont.)

2166	C7H15O2-3=C7H14-3+HO2	1.00E+39	-8.11	41490	
2167	C7H15O2-4=C7H14-3+HO2	2.01E+39	-8.11	41490	
2168	C7H15O2-1=C7H14OOH1-2	2.00E+11	0	26450	
2169	C7H15O2-1=C7H14OOH1-3	2.50E+10	0	20450	
2170	C7H15O2-1=C7H14OOH1-4	3.13E+09	0	18650	
2171	C7H15O2-1=C7H14OOH1-5	3.91E+08	0	21650	
2172	C7H15O2-2=C7H14OOH2-1	3.00E+11	0	29000	
2173	C7H15O2-2=C7H14OOH2-3	2.00E+11	0	26450	
2174	C7H15O2-2=C7H14OOH2-4	2.50E+10	0	20450	
2175	C7H15O2-2=C7H14OOH2-5	3.13E+09	0	18650	
2176	C7H15O2-2=C7H14OOH2-6	3.91E+08	0	21650	
2177	C7H15O2-3=C7H14OOH3-1	3.75E+10	0	24000	
2178	C7H15O2-3=C7H14OOH3-2	2.00E+11	0	26450	
2179	C7H15O2-3=C7H14OOH3-4	2.00E+11	0	26450	
2180	C7H15O2-3=C7H14OOH3-5	2.50E+10	0	20450	
2181	C7H15O2-3=C7H14OOH3-6	3.13E+09	0	18650	
2182	C7H15O2-3=C7H14OOH3-7	5.86E+08	0	25150	
2183	C7H15O2-4=C7H14OOH4-1	9.38E+09	0	21950	
2184	C7H15O2-4=C7H14OOH4-2	5.00E+10	0	20450	
2185	C7H15O2-4=C7H14OOH4-3	4.00E+11	0	26450	REV/3.782E13 -7.9E-1 3.401E4/
2186	C7H15O2-1+HO2=C7H15O2H-1+O2	1.75E+10	0	-3275	REV/4.496E13 -8.2E-1 3.404E4/
2187	C7H15O2-2+HO2=C7H15O2H-2+O2	1.75E+10	0	-3275	REV/4.496E13 -8.2E-1 3.404E4/
2188	C7H15O2-3+HO2=C7H15O2H-3+O2	1.75E+10	0	-3275	REV/4.497E13 -8.2E-1 3.404E4/
2189	C7H15O2-4+HO2=C7H15O2H-4+O2	1.75E+10	0	-3275	REV/2.4E12 0.0E0 1.0E4/
2190	H2O2+C7H15O2-1=HO2+C7H15O2H-1	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
2191	H2O2+C7H15O2-2=HO2+C7H15O2H-2	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
2192	H2O2+C7H15O2-3=HO2+C7H15O2H-3	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
2193	H2O2+C7H15O2-4=HO2+C7H15O2H-4	2.40E+12	0	10000	
2194	C7H15O2-1+CH3O2=>C7H15O-1+CH3O+O2	1.40E+16	-1.61	1860	
2195	C7H15O2-2+CH3O2=>C7H15O-2+CH3O+O2	1.40E+16	-1.61	1860	
2196	C7H15O2-3+CH3O2=>C7H15O-3+CH3O+O2	1.40E+16	-1.61	1860	
2197	C7H15O2-4+CH3O2=>C7H15O-4+CH3O+O2	1.40E+16	-1.61	1860	
2198	2C7H15O2-1=>O2+2C7H15O-1	1.40E+16	-1.61	1860	
2199	C7H15O2-1+C7H15O2-2=>C7H15O-1+C7H15O-2+O2	1.40E+16	-1.61	1860	
2200	C7H15O2-1+C7H15O2-3=>C7H15O-1+C7H15O-3+O2	1.40E+16	-1.61	1860	
2201	C7H15O2-1+C7H15O2-4=>C7H15O-1+C7H15O-4+O2	1.40E+16	-1.61	1860	
2202	2C7H15O2-2=>O2+2C7H15O-2	1.40E+16	-1.61	1860	
2203	C7H15O2-2+C7H15O2-3=>C7H15O-2+C7H15O-3+O2	1.40E+16	-1.61	1860	
2204	C7H15O2-2+C7H15O2-4=>C7H15O-2+C7H15O-4+O2	1.40E+16	-1.61	1860	
2205	2C7H15O2-3=>O2+2C7H15O-3	1.40E+16	-1.61	1860	
2206	C7H15O2-3+C7H15O2-4=>C7H15O-3+C7H15O-4+O2	1.40E+16	-1.61	1860	
2207	2C7H15O2-4=>O2+2C7H15O-4	1.40E+16	-1.61	1860	REV/1.989E7 1.93E0 -6.522E3/
2208	C7H15O2H-1=C7H15O-1+OH	1.00E+16	0	39000	REV/9.517E6 2.03E0 -6.922E3/
2209	C7H15O2H-2=C7H15O-2+OH	1.00E+16	0	39000	REV/9.517E6 2.03E0 -6.922E3/
2210	C7H15O2H-3=C7H15O-3+OH	1.00E+16	0	39000	REV/9.516E6 2.03E0 -6.922E3/

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Table B .1. (cont.)

2211	C7H15O2H-4=C7H15O-4+OH	1.00E+16	0	39000	REV/1.0E11 0.0E0 1.19E4/
2212	C7H15O-1=CH2O+C6H13-1	6.02E+20	-2.18	24830	REV/1.0E11 0.0E0 1.29E4/
2213	C7H15O-2=CH3CHO+C5H11-1	1.48E+22	-2.55	20370	REV/1.0E11 0.0E0 1.29E4/
2214	C7H15O-3=C2H5CHO+PC4H9	6.57E+17	-1.16	19370	REV/1.0E11 0.0E0 1.29E4/
2215	C7H15O-4=NC3H7CHO+NC3H7	4.77E+22	-2.58	21820	
2216	C7H14-1+HO2=C7H14OOH1-2	2.50E+03	2.5	11200	
2217	C7H14-1+HO2=C7H14OOH2-1	2.70E+03	2.5	10500	
2218	C7H14-2+HO2=C7H14OOH2-3	2.70E+03	2.5	10500	
2219	C7H14-2+HO2=C7H14OOH3-2	2.70E+03	2.5	10500	
2220	C7H14-3+HO2=C7H14OOH3-4	2.70E+03	2.5	10500	
2221	C7H14-3+HO2=C7H14OOH4-3	2.70E+03	2.5	10500	
2222	C7H14OOH1-2=>C7H14O1-2+OH	6.00E+11	0	22000	
2223	C7H14OOH1-3=>C7H14O1-3+OH	7.50E+10	0	15250	
2224	C7H14OOH1-4=>C7H14O1-4+OH	9.38E+09	0	7000	
2225	C7H14OOH1-5=>C7H14O1-5+OH	1.17E+09	0	1800	
2226	C7H14OOH2-1=>C7H14O1-2+OH	6.00E+11	0	22000	
2227	C7H14OOH2-3=>C7H14O2-3+OH	6.00E+11	0	22000	
2228	C7H14OOH2-4=>C7H14O2-4+OH	7.50E+10	0	15250	
2229	C7H14OOH2-5=>C7H14O2-5+OH	9.38E+09	0	7000	
2230	C7H14OOH2-6=>C7H14O2-6+OH	1.17E+09	0	1800	
2231	C7H14OOH3-1=>C7H14O1-3+OH	7.50E+10	0	15250	
2232	C7H14OOH3-2=>C7H14O2-3+OH	6.00E+11	0	22000	
2233	C7H14OOH3-4=>C7H14O3-4+OH	6.00E+11	0	22000	
2234	C7H14OOH3-5=>C7H14O3-5+OH	7.50E+10	0	15250	
2235	C7H14OOH3-6=>C7H14O2-5+OH	9.38E+09	0	7000	
2236	C7H14OOH3-7=>C7H14O1-5+OH	1.17E+09	0	1800	
2237	C7H14OOH4-1=>C7H14O1-4+OH	9.38E+09	0	7000	
2238	C7H14OOH4-2=>C7H14O2-4+OH	7.50E+10	0	15250	
2239	C7H14OOH4-3=>C7H14O3-4+OH	6.00E+11	0	22000	
2240	C7H14OOH1-3=>OH+CH2O+C6H12-1	2.15E+09	1.23	30370	
2241	C7H14OOH2-4=>OH+CH3CHO+C5H10-1	1.55E+12	0.59	30090	
2242	C7H14OOH3-1=>OH+NC4H9CHO+C2H4	8.18E+13	-0.13	31330	
2243	C7H14OOH3-5=>OH+C2H5CHO+C4H8-1	2.66E+13	0.13	30430	
2244	C7H14OOH4-2=>OH+NC3H7CHO+C3H6	6.19E+13	0.09	30840	REV/2.2E3 2.48E0 6.13E3/
2245	C7H14OOH1-3=C4H7OOH1-4+NC3H7	1.61E+12	0.54	27740	
2246	C7H14OOH1-4=>C5H10-1+C2H4+HO2	1.45E+11	0.69	30820	REV/2.2E3 2.48E0 6.13E3/
2247	C7H14OOH1-4=C5H9OOH1-5+C2H5	1.72E+12	0.51	27900	REV/2.2E3 2.48E0 6.13E3/
2248	C7H14OOH2-4=C5H9OOH1-4+C2H5	4.08E+12	0.32	29230	REV/2.2E3 2.48E0 6.13E3/
2249	C7H14OOH2-5=C4H8-1+C3H6OOH2-1	6.86E+13	0.03	31380	REV/2.2E3 2.48E0 6.13E3/
2250	C7H14OOH2-5=C6H11OOH1-5+CH3	7.42E+10	0.75	30260	REV/2.2E3 2.48E0 6.13E3/
2251	C7H14OOH3-5=C6H11OOH1-4+CH3	7.42E+10	0.75	30260	REV/2.2E3 2.48E0 6.13E3/
2252	C7H14OOH3-6=C4H8OOH2-1+C3H6	4.58E+11	0.6	29170	REV/2.2E3 2.48E0 6.13E3/
2253	C7H14OOH4-1=C5H10OOH2-1+C2H4	1.64E+12	0.44	29320	REV/7.54E12 0.0E0 0.0E0/
2254	C7H14OOH1-2O2=C7H14OOH1-2+O2	1.37E+23	-2.37	37640	REV/7.54E12 0.0E0 0.0E0/
2255	C7H14OOH1-3O2=C7H14OOH1-3+O2	1.37E+23	-2.37	37640	REV/7.54E12 0.0E0 0.0E0/
2256	C7H14OOH1-4O2=C7H14OOH1-4+O2	1.37E+23	-2.37	37640	REV/7.54E12 0.0E0 0.0E0/
2257	C7H14OOH1-5O2=C7H14OOH1-5+O2	1.37E+23	-2.37	37640	REV/4.52E12 0.0E0 0.0E0/
2258	C7H14OOH2-1O2=C7H14OOH2-1+O2	3.32E+20	-1.65	35280	REV/7.54E12 0.0E0 0.0E0/

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Table B .1. (cont.)

2259	C7H14OOH2-3O2=C7H14OOH2-3+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2260	C7H14OOH2-4O2=C7H14OOH2-4+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2261	C7H14OOH2-5O2=C7H14OOH2-5+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2262	C7H14OOH2-6O2=C7H14OOH2-6+O2	1.39E+23	-2.38	37600	REV/4.52E12 0.0E0 0.0E0/
2263	C7H14OOH3-1O2=C7H14OOH3-1+O2	3.32E+20	-1.65	35280	REV/7.54E12 0.0E0 0.0E0/
2264	C7H14OOH3-2O2=C7H14OOH3-2+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2265	C7H14OOH3-4O2=C7H14OOH3-4+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2266	C7H14OOH3-5O2=C7H14OOH3-5+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2267	C7H14OOH3-6O2=C7H14OOH3-6+O2	1.39E+23	-2.38	37600	REV/4.52E12 0.0E0 0.0E0/
2268	C7H14OOH3-7O2=C7H14OOH3-7+O2	3.32E+20	-1.65	35280	REV/4.52E12 0.0E0 0.0E0/
2269	C7H14OOH4-1O2=C7H14OOH4-1+O2	1.67E+20	-1.65	35280	REV/7.54E12 0.0E0 0.0E0/
2270	C7H14OOH4-2O2=C7H14OOH4-2+O2	6.97E+22	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
2271	C7H14OOH4-3O2=C7H14OOH4-3+O2	6.97E+22	-2.38	37600	
2272	C7H14OOH1-2O2=NC7KET12+OH	2.00E+11	0	26000	
2273	C7H14OOH1-3O2=NC7KET13+OH	2.50E+10	0	21000	
2274	C7H14OOH1-4O2=NC7KET14+OH	3.13E+09	0	18950	
2275	C7H14OOH1-5O2=NC7KET15+OH	3.91E+08	0	22150	
2276	C7H14OOH2-1O2=NC7KET21+OH	1.00E+11	0	23450	
2277	C7H14OOH2-3O2=NC7KET23+OH	1.00E+11	0	23450	
2278	C7H14OOH2-4O2=NC7KET24+OH	1.25E+10	0	17450	
2279	C7H14OOH2-5O2=NC7KET25+OH	1.56E+09	0	15650	
2280	C7H14OOH2-6O2=NC7KET26+OH	1.95E+08	0	18650	
2281	C7H14OOH3-1O2=NC7KET31+OH	1.25E+10	0	17450	
2282	C7H14OOH3-2O2=NC7KET32+OH	1.00E+11	0	23450	
2283	C7H14OOH3-4O2=NC7KET34+OH	1.00E+11	0	23450	
2284	C7H14OOH3-5O2=NC7KET35+OH	1.25E+10	0	17450	
2285	C7H14OOH3-6O2=NC7KET36+OH	1.56E+09	0	15650	
2286	C7H14OOH3-7O2=NC7KET37+OH	1.95E+08	0	18650	
2287	C7H14OOH4-1O2=NC7KET41+OH	1.56E+09	0	15650	
2288	C7H14OOH4-2O2=NC7KET42+OH	1.25E+10	0	17450	
2289	C7H14OOH4-3O2=NC7KET43+OH	1.00E+11	0	23450	
2290	NC7KET12=>NC5H11CHO+HCO+OH	1.00E+16	0	39000	
2291	NC7KET13=>NC4H9CHO+CH2CHO+OH	1.00E+16	0	39000	
2292	NC7KET14=>NC3H7CHO+CH2CH2CHO+OH	1.00E+16	0	39000	
2293	NC7KET15=>C2H5CHO+C3H6CHO-1+OH	1.00E+16	0	39000	
2294	NC7KET21=>CH2O+NC5H11CO+OH	1.00E+16	0	39000	
2295	NC7KET23=>NC4H9CHO+CH3CO+OH	1.00E+16	0	39000	
2296	NC7KET24=>NC3H7CHO+CH3COCH2+OH	1.00E+16	0	39000	
2297	NC7KET25=>C2H5CHO+CH2CH2COCH3+OH	1.00E+16	0	39000	
2298	NC7KET26=>CH3CHO+C3H6COCH3-1+OH	1.00E+16	0	39000	
2299	NC7KET31=>CH2O+NC4H9COCH2+OH	1.00E+16	0	39000	
2300	NC7KET32=>CH3CHO+NC4H9CO+OH	1.00E+16	0	39000	
2301	NC7KET34=>NC3H7CHO+C2H5CO+OH	1.00E+16	0	39000	
2302	NC7KET35=>C2H5CHO+C2H5COCH2+OH	1.00E+16	0	39000	
2303	NC7KET36=>CH3CHO+C2H5COC2H4P+OH	1.00E+16	0	39000	
2304	NC7KET37=>CH2O+C3H6COC2H5-1+OH	1.00E+16	0	39000	
2305	NC7KET41=>CH2O+NC3H7COC2H4P+OH	1.00E+16	0	39000	
2306	NC7KET42=>CH3CHO+NC3H7COCH2+OH	1.00E+16	0	39000	

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Table B .1. (cont.)

2307	NC7KET43=>C2H5CHO+NC3H7CO+OH	1.00E+16	0	39000	
2308	C7H14O1-2+OH=>PC4H9+C2H3CHO+H2O	2.50E+12	0	0	
2309	C7H14O1-3+OH=>C6H12-1+HCO+H2O	2.50E+12	0	0	
2310	C7H14O1-4+OH=>C5H10-1+CH2CHO+H2O	2.50E+12	0	0	
2311	C7H14O1-5+OH=>C4H8-1+CH2CH2CHO+H2O	2.50E+12	0	0	
2312	C7H14O2-3+OH=>C2H3COCH3+NC3H7+H2O	2.50E+12	0	0	
2313	C7H14O2-4+OH=>CH3CO+C5H10-1+H2O	2.50E+12	0	0	
2314	C7H14O2-5+OH=>CH3COCH2+C4H8-1+H2O	2.50E+12	0	0	
2315	C7H14O2-6+OH=>CH2CH2COCH3+C3H6+H2O	2.50E+12	0	0	
2316	C7H14O3-4+OH=>C2H5COC2H3+C2H5+H2O	2.50E+12	0	0	
2317	C7H14O3-5+OH=>C2H5CO+C4H8-1+H2O	2.50E+12	0	0	
2318	C7H14O1-2+OH=>CH2CO+C5H11-1+H2O	2.50E+12	0	0	
2319	C7H14O1-3+OH=>C2H4+NC4H9CO+H2O	2.50E+12	0	0	
2320	C7H14O1-4+OH=>C2H4+NC3H7COCH2+H2O	2.50E+12	0	0	
2321	C7H14O1-5+OH=>C2H4+C2H5COC2H4P+H2O	2.50E+12	0	0	
2322	C7H14O2-3+OH=>CH3CHCO+PC4H9+H2O	2.50E+12	0	0	
2323	C7H14O2-4+OH=>C3H6+NC3H7CO+H2O	2.50E+12	0	0	
2324	C7H14O2-5+OH=>C3H6+C2H5COCH2+H2O	2.50E+12	0	0	
2325	C7H14O2-6+OH=>CH3CHO+C5H91-4+H2O	2.50E+12	0	0	
2326	C7H14O3-4+OH=>C2H5CHCO+NC3H7+H2O	2.50E+12	0	0	
2327	C7H14O3-5+OH=>C2H5CHO+C4H71-2+H2O	2.50E+12	0	0	
2328	C7H14O1-2+HO2=>PC4H9+C2H3CHO+H2O2	5.00E+12	0	17700	
2329	C7H14O1-3+HO2=>C6H12-1+HCO+H2O2	5.00E+12	0	17700	
2330	C7H14O1-4+HO2=>C5H10-1+CH2CHO+H2O2	5.00E+12	0	17700	
2331	C7H14O1-5+HO2=>C4H8-1+CH2CH2CHO+H2O2	5.00E+12	0	17700	
2332	C7H14O2-3+HO2=>C2H3COCH3+NC3H7+H2O2	5.00E+12	0	17700	
2333	C7H14O2-4+HO2=>CH3CO+C5H10-1+H2O2	5.00E+12	0	17700	
2334	C7H14O2-5+HO2=>CH3COCH2+C4H8-1+H2O2	5.00E+12	0	17700	
2335	C7H14O2-6+HO2=>CH2CH2COCH3+C3H6+H2O2	5.00E+12	0	17700	
2336	C7H14O3-4+HO2=>C2H5COC2H3+C2H5+H2O2	5.00E+12	0	17700	
2337	C7H14O3-5+HO2=>C2H5CO+C4H8-1+H2O2	5.00E+12	0	17700	
2338	C7H14O1-2+HO2=>CH2CO+C5H11-1+H2O2	5.00E+12	0	17700	
2339	C7H14O1-3+HO2=>C2H4+NC4H9CO+H2O2	5.00E+12	0	17700	
2340	C7H14O1-4+HO2=>C2H4+NC3H7COCH2+H2O2	5.00E+12	0	17700	
2341	C7H14O1-5+HO2=>C2H4+C2H5COC2H4P+H2O2	5.00E+12	0	17700	
2342	C7H14O2-3+HO2=>CH3CHCO+PC4H9+H2O2	5.00E+12	0	17700	
2343	C7H14O2-4+HO2=>C3H6+NC3H7CO+H2O2	5.00E+12	0	17700	
2344	C7H14O2-5+HO2=>C3H6+C2H5COCH2+H2O2	5.00E+12	0	17700	
2345	C7H14O2-6+HO2=>CH3CHO+C5H91-4+H2O2	5.00E+12	0	17700	
2346	C7H14O3-4+HO2=>C2H5CHCO+NC3H7+H2O2	5.00E+12	0	17700	
2347	C7H14O3-5+HO2=>C2H5CHO+C4H71-2+H2O2	5.00E+12	0	17700	REV/1.0E12 0.0E0 -1.042E3/
2348	C7H14OH-1=C7H14-1+OH	5.43E+14	-0.53	27830	REV/2.0E12 0.0E0 0.0E0/
2349	O2C7H14OH-1=C7H14OH-1+O2	2.98E+21	-1.98	37820	
2350	O2C7H14OH-1=>NC5H11CHO+CH2O+OH	2.50E+10	0	18860	REV/1.0E12 0.0E0 -1.042E3/
2351	C7H14OH-2=C7H14-2+OH	1.04E+16	-1	29400	REV/2.0E12 0.0E0 0.0E0/
2352	O2C7H14OH-2=C7H14OH-2+O2	4.78E+21	-2.06	37860	
2353	O2C7H14OH-1=>NC4H9CHO+CH3CHO+OH	2.50E+10	0	18860	REV/1.0E12 0.0E0 -1.042E3/

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Table B .1. (cont.)

2354	C7H14OH-3=C7H14-3+OH	7.77E+15	-0.93	29490	REV/2.0E12 0.0E0 0.0E0/
2355	O2C7H14OH-3=C7H14OH-3+O2	4.78E+21	-2.06	37860	
2356	O2C7H14OH-3=>NC3H7CHO+C2H5CHO+OH	2.50E+10	0	18860	REV/1.0E7 0.0E0 4.0E4/
2357	NC5H11CHO+O2=NC5H11CO+HO2	2.00E+13	0.5	42200	REV/1.74E10 7.6E-1 3.12E4/
2358	NC5H11CHO+OH=NC5H11CO+H2O	2.69E+10	0.76	-340	REV/1.8E13 0.0E0 2.4E4/
2359	NC5H11CHO+H=NC5H11CO+H2	4.00E+13	0	4200	REV/1.0E12 0.0E0 1.9E4/
2360	NC5H11CHO+O=NC5H11CO+OH	5.00E+12	0	1790	REV/1.0E12 0.0E0 1.0E4/
2361	NC5H11CHO+HO2=NC5H11CO+H2O2	2.80E+12	0	13600	REV/1.5E13 0.0E0 2.8E4/
2362	NC5H11CHO+CH3=NC5H11CO+CH4	1.70E+12	0	8440	REV/3.0E11 0.0E0 1.8E4/
2363	NC5H11CHO+CH3O=NC5H11CO+CH3OH	1.15E+11	0	1280	REV/2.5E10 0.0E0 1.0E4/
2364	NC5H11CHO+CH3O2=NC5H11CO+CH3O2H	1.00E+12	0	9500	REV/1.071E9 9.6E-1 2.101E4/
2365	NC5H11CHO+OH=C5H10CHO-1+H2O	5.27E+09	0.97	1586	REV/1.752E6 1.85E0 2.388E4/
2366	NC5H11CHO+OH=C5H10CHO-2+H2O	4.67E+07	1.61	-35	REV/1.752E6 1.85E0 2.388E4/
2367	NC5H11CHO+OH=C5H10CHO-3+H2O	4.67E+07	1.61	-35	REV/1.752E6 1.85E0 2.388E4/
2368	NC5H11CHO+OH=C5H10CHO-4+H2O	4.67E+07	1.61	-35	REV/3.317E9 1.25E0 3.084E4/
2369	NC5H11CHO+OH=C5H10CHO-5+H2O	4.67E+07	1.61	-35	REV/1.0E11 0.0E0 0.0E0/
2370	NC5H11CO=C5H11-1+CO	1.00E+11	0	9600	REV/3.33E4 2.22E0 4.442E3/
2371	NC5H11CHO+HO2=C5H10CHO-1+H2O2	2.76E+04	2.55	16480	REV/3.285E3 2.51E0 6.362E3/
2372	NC5H11CHO+HO2=C5H10CHO-2+H2O2	1.48E+04	2.6	13910	REV/3.285E3 2.51E0 6.362E3/
2373	NC5H11CHO+HO2=C5H10CHO-3+H2O2	1.48E+04	2.6	13910	REV/3.285E3 2.51E0 6.362E3/
2374	NC5H11CHO+HO2=C5H10CHO-4+H2O2	1.48E+04	2.6	13910	REV/1.244E7 1.91E0 1.332E4/
2375	NC5H11CHO+HO2=C5H10CHO-5+H2O2	2.95E+04	2.6	13910	REV/2.99E13 -5.1E-1 6.617E3/
2376	NC5H11CHO+CH3O2=C5H10CHO-1+CH3O2H	6.03E+12	0	19380	REV/1.821E12 -2.6E-1 8.784E3/
2377	NC5H11CHO+CH3O2=C5H10CHO-2+CH3O2H	1.99E+12	0	17050	REV/1.821E12 -2.6E-1 8.784E3/
2378	NC5H11CHO+CH3O2=C5H10CHO-3+CH3O2H	1.99E+12	0	17050	REV/1.821E12 -2.6E-1 8.784E3/
2379	NC5H11CHO+CH3O2=C5H10CHO-4+CH3O2H	1.99E+12	0	17050	REV/6.897E15 -8.6E-1 1.574E4/
2380	NC5H11CHO+CH3O2=C5H10CHO-5+CH3O2H	3.98E+12	0	17050	REV/2.5E11 0.0E0 7.8E3/
2381	C5H10CHO-1=C2H4+C3H6CHO-1	2.68E+18	-1.58	30410	REV/1.0E11 0.0E0 7.8E3/
2382	C5H10CHO-2=C3H6+CH2CH2CHO	9.38E+17	-1.31	31970	REV/1.0E11 0.0E0 7.8E3/
2383	C5H10CHO-3=C4H8-1+CH2CHO	6.27E+16	-1.43	25990	REV/1.0E11 0.0E0 7.8E3/
2384	C5H10CHO-3=C4H7CHO1-4+CH3	2.37E+14	-0.56	31320	REV/1.0E11 0.0E0 7.8E3/
2385	C5H10CHO-4=AC3H5CHO+C2H5	7.19E+17	-1.37	33230	REV/1.0E11 0.0E0 7.8E3/
2386	C5H10CHO-4=C5H10-1+HCO	1.06E+14	-0.41	26330	REV/1.0E11 0.0E0 7.8E3/
2387	C5H10CHO-5=C2H3CHO+NC3H7	1.56E+19	-1.53	33310	REV/2.398E12 -2.0E-2 3.094E4/
2388	C4H7CHO1-4+OH=C4H7CO1-4+H2O	3.37E+12	0	-616	REV/1.187E8 1.74E0 3.498E4/
2389	C4H7CHO1-4+OH=C4H6CHO1-43+H2O	2.08E+06	2	-298	REV/1.502E9 1.31E0 2.89E4/
2390	C4H7CHO1-4+OH=C4H6CHO1-44+H2O	4.67E+07	1.61	-35	REV/5.344E6 9.7E-1 1.926E4/
2391	C4H7CHO1-4+OH=CH3CHO+CH2CH2CHO	1.00E+11	0	0	REV/4.225E12 -3.5E-1 1.201E4/
2392	C4H7CHO1-4+HO2=C4H7CO1-4+H2O2	1.00E+12	0	11920	REV/3.265E6 2.01E0 1.773E4/
2393	C4H7CHO1-4+HO2=C4H6CHO1-43+H2O2	9.64E+03	2.6	13910	REV/2.815E6 1.97E0 1.138E4/

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Table B .1. (cont.)

2394	C4H7CHO1-4+HO2=C4H6CHO1-44+H2O2	1.48E+04	2.6	13910	REV/4.861E13 -5.2E-1 1.297E4/
2395	C4H7CHO1-4+CH3O2=C4H7CO1-4+CH3O2H	2.80E+12	0	13600	REV/2.77E15 -7.7E-1 2.015E4/
2396	C4H7CHO1-4+CH3O2=C4H6CHO1-43+CH3O2H	1.99E+12	0	17050	REV/1.561E15 -8.0E-1 1.38E4/
2397	C4H7CHO1-4+CH3O2=C4H6CHO1-44+CH3O2H	1.99E+12	0	17050	REV/1.5E11 0.0E0 4.81E3/
2398	C4H7CO1-4=C4H71-4+CO	7.37E+18	-1.76	15230	REV/1.0E11 0.0E0 7.8E3/
2399	C4H6CHO1-43=C4H6+HCO	4.83E+15	-0.79	33540	REV/1.0E11 0.0E0 7.8E3/
2400	C4H6CHO1-44=C2H3CHO+C2H3	2.12E+14	-0.39	37160	REV/4.278E6 1.72E0 2.019E4/
2401	NC4H9COCH3+OH=C4H8COCH3-1+H2O	2.07E+07	1.73	753	REV/3.07E5 2.04E0 2.163E4/
2402	NC4H9COCH3+OH=C4H8COCH3-2+H2O	3.62E+07	1.64	-247	REV/3.07E5 2.04E0 2.163E4/
2403	NC4H9COCH3+OH=C4H8COCH3-3+H2O	3.62E+07	1.64	-247	REV/1.633E13 -2.3E-1 2.864E4/
2404	NC4H9COCH3+OH=C4H8COCH3-4+H2O	8.45E+11	0	-228	REV/6.786E13 -7.0E-1 2.768E4/
2405	NC4H9COCH3+OH=NC4H9COCH2+H2O	5.10E+11	0	1192	REV/2.927E4 2.21E0 4.462E3/
2406	NC4H9COCH3+HO2=C4H8COCH3-1+H2O2	2.38E+04	2.55	16490	REV/2.823E11 7.0E-2 8.112E3/
2407	NC4H9COCH3+HO2=C4H8COCH3-2+H2O2	5.60E+12	0	17700	REV/2.823E11 7.0E-2 8.112E3/
2408	NC4H9COCH3+HO2=C4H8COCH3-3+H2O2	5.60E+12	0	17700	REV/2.294E13 -5.6E-1 6.1E3/
2409	NC4H9COCH3+HO2=C4H8COCH3-4+H2O2	2.00E+11	0	8698	REV/1.88E7 1.52E0 9.712E3/
2410	NC4H9COCH3+HO2=NC4H9COCH2+H2O2	2.38E+04	2.55	14690	REV/1.521E13 -5.1E-1 6.627E3/
2411	NC4H9COCH3+CH3O2=C4H8COCH3-1+CH3O2H	3.01E+12	0	19380	REV/4.123E11 -1.1E-1 6.744E3/
2412	NC4H9COCH3+CH3O2=C4H8COCH3-2+CH3O2H	1.99E+12	0	17050	REV/4.123E11 -1.1E-1 6.744E3/
2413	NC4H9COCH3+CH3O2=C4H8COCH3-3+CH3O2H	1.99E+12	0	17050	REV/9.429E14 -7.3E-1 1.193E4/
2414	NC4H9COCH3+CH3O2=C4H8COCH3-4+CH3O2H	2.00E+12	0	15250	REV/9.77E15 -1.21E0 1.188E4/
2415	NC4H9COCH3+CH3O2=NC4H9COCH2+CH3O2H	3.01E+12	0	17580	REV/1.0E11 0.0E0 8.3E3/
2416	C4H8COCH3-1=CH2CH2COCH3+C2H4	1.13E+18	-1.59	30910	REV/1.0E11 0.0E0 8.3E3/
2417	C4H8COCH3-2=C3H6+CH3COCH2	3.18E+15	-0.79	26220	REV/1.0E11 0.0E0 9.8E3/
2418	C4H8COCH3-3=C4H8-1+CH3CO	1.71E+18	-1.61	28250	REV/1.0E11 0.0E0 8.3E3/
2419	C4H8COCH3-4=C2H3COCH3+C2H5	4.69E+19	-1.61	33750	REV/1.0E11 0.0E0 1.16E4/
2420	NC4H9COCH2=PC4H9+CH2CO	1.55E+18	-1.41	43140	REV/2.0E13 0.0E0 0.0E0/
2421	C4H7OOH1-4=C4H7O1-4+OH	2.02E+20	-1.53	47040	REV/2.0E13 0.0E0 0.0E0/
2422	C5H9OOH1-4=C5H9O1-4+OH	1.18E+20	-1.38	46050	REV/2.0E13 0.0E0 0.0E0/
2423	C5H9OOH1-5=C5H9O1-5+OH	1.59E+20	-1.5	46990	REV/2.0E13 0.0E0 0.0E0/
2424	C6H11OOH1-4=C6H11O1-4+OH	1.23E+20	-1.39	46050	REV/2.0E13 0.0E0 0.0E0/
2425	C6H11OOH1-5=C6H11O1-5+OH	1.23E+20	-1.39	46050	REV/1.0E11 0.0E0 1.19E4/
2426	C4H7O1-4=CH2O+C3H5-A	2.41E+16	-1.14	7550	REV/5.0E10 0.0E0 9.6E3/
2427	C5H9O1-4=CH3CHO+C3H5-A	7.72E+20	-2.43	5890	REV/1.0E11 0.0E0 9.6E3/
2428	C5H9O1-4=AC3H5CHO+CH3	1.11E+17	-1.21	17960	REV/1.0E11 0.0E0 9.6E3/
2429	C5H9O1-5=CH2O+C4H71-4	4.31E+17	-1.33	17940	REV/1.0E11 0.0E0 9.6E3/
2430	C6H11O1-4=AC3H5CHO+C2H5	7.27E+20	-2.1	18870	REV/5.0E10 0.0E0 9.6E3/
2431	C6H11O1-4=C2H5CHO+C3H5-A	1.21E+21	-2.46	5641	REV/1.0E11 0.0E0 9.6E3/
2432	C6H11O1-5=C4H7CHO1-4+CH3	2.40E+17	-1.3	16960	REV/1.0E11 0.0E0 9.6E3/
2433	C6H11O1-5=CH3CHO+C4H71-4	2.00E+22	-2.58	18530	REV/2.0E11 0.0E0 7.8E3/
2434	C5H91-1=C2H2+NC3H7	2.76E+15	-0.67	30800	REV/5.203E12 3.0E-2 3.68E4/

(cont. on next page)

Table B .1. (cont.)

2435	C4H7CHO1-1+OH=C4H7CO1-1+H2O	3.37E+12	0	-616	REV/1.067E9 9.6E-1 2.102E4/
2436	C4H7CHO1-1+OH=C4H6CHO1-14+H2O	5.27E+09	0.97	1586	REV/1.251E8 1.79E0 3.493E4/
2437	C4H7CHO1-1+OH=C4H6CHO1-13+H2O	3.12E+06	2	-298	REV/1.076E7 1.1E0 1.702E4/
2438	C4H7CHO1-1+OH=C2H5CHO+CH2CHO	1.00E+11	0	0	REV/9.165E12 -3.0E-1 1.787E4/
2439	C4H7CHO1-1+HO2=C4H7CO1-1+H2O2	1.00E+12	0	11920	REV/3.317E4 2.22E0 4.452E3/
2440	C4H7CHO1-1+HO2=C4H6CHO1-14+H2O2	2.76E+04	2.55	16480	REV/2.295E6 2.06E0 1.768E4/
2441	C4H7CHO1-1+HO2=C4H6CHO1-13+H2O2	9.64E+03	2.6	13910	REV/1.055E14 -4.7E-1 1.883E4/
2442	C4H7CHO1-1+CH3O2=C4H7CO1-1+CH3O2H	2.80E+12	0	13600	REV/2.978E13 -5.1E-1 6.627E3/
2443	C4H7CHO1-1+CH3O2=C4H6CHO1-14+CH3O2H	6.03E+12	0	19380	REV/1.947E15 -7.2E-1 2.01E4/
2444	C4H7CHO1-1+CH3O2=C4H6CHO1-13+CH3O2H	1.99E+12	0	17050	REV/1.5E11 0.0E0 4.81E3/
2445	C4H7CO1-1=C4H71-1+CO	8.51E+20	-2.12	40320	REV/8.0E10 0.0E0 1.14E4/
2446	C4H6CHO1-14=C2H4+CHCHCHO	9.05E+16	-1.33	46870	REV/8.0E10 0.0E0 1.14E4/
2447	C4H6CHO1-13=C4H6+HCO	8.95E+17	-1.28	46230	REV/5.173E6 1.7E0 2.022E4/
2448	NC3H7COC2H5+OH=C3H6COC2H5-1+H2O	2.07E+07	1.73	753	REV/7.233E5 1.92E0 2.176E4/
2449	NC3H7COC2H5+OH=C3H6COC2H5-2+H2O	3.62E+07	1.64	-247	REV/3.313E13 -3.2E-1 2.874E4/
2450	NC3H7COC2H5+OH=C3H6COC2H5-3+H2O	8.45E+11	0	-228	REV/1.278E11 -3.0E-2 2.066E4/
2451	NC3H7COC2H5+OH=NC3H7COC2H4P+H2O	5.10E+11	0	1192	REV/3.313E13 -3.2E-1 2.874E4/
2452	NC3H7COC2H5+OH=NC3H7COC2H4S+H2O	8.45E+11	0	-228	REV/3.539E4 2.19E0 4.492E3/
2453	NC3H7COC2H5+HO2=C3H6COC2H5-1+H2O2	2.38E+04	2.55	16490	REV/6.652E11 -5.0E-2 8.242E3/
2454	NC3H7COC2H5+HO2=C3H6COC2H5-2+H2O2	5.60E+12	0	17700	REV/4.654E13 -6.5E-1 6.2E3/
2455	NC3H7COC2H5+HO2=C3H6COC2H5-3+H2O2	2.00E+11	0	8698	REV/3.539E4 2.19E0 2.692E3/
2456	NC3H7COC2H5+HO2=NC3H7COC2H4P+H2O2	2.38E+04	2.55	14690	REV/4.654E13 -6.5E-1 6.2E3/
2457	NC3H7COC2H5+HO2=NC3H7COC2H4S+H2O2	2.00E+11	0	8698	REV/1.839E13 -5.4E-1 6.657E3/
2458	NC3H7COC2H5+CH3O2=C3H6COC2H5-1+CH3O2H	3.01E+12	0	19380	REV/9.713E11 -2.2E-1 6.874E3/
2459	NC3H7COC2H5+CH3O2=C3H6COC2H5-2+CH3O2H	1.99E+12	0	17050	REV/1.913E15 -8.3E-1 1.203E4/
2460	NC3H7COC2H5+CH3O2=C3H6COC2H5-3+CH3O2H	2.00E+12	0	15250	REV/1.839E13 -5.4E-1 4.862E3/
2461	NC3H7COC2H5+CH3O2=NC3H7COC2H4P+CH3O2H	3.01E+12	0	17580	REV/1.913E15 -8.3E-1 1.203E4/
2462	NC3H7COC2H5+CH3O2=NC3H7COC2H4S+CH3O2H	2.00E+12	0	15250	REV/2.5E11 0.0E0 7.8E3/
2463	C3H6COC2H5-1=C2H4+C2H5COCH2	2.22E+15	-0.84	23590	REV/1.0E11 0.0E0 8.3E3/
2464	C3H6COC2H5-2=C3H6+C2H5CO	4.05E+16	-1.11	26150	REV/1.0E11 0.0E0 7.8E3/
2465	C3H6COC2H5-3=C2H5COC2H3+CH3	2.92E+15	-0.68	32300	REV/2.5E11 0.0E0 7.8E3/
2466	NC3H7COC2H4P=NC3H7CO+C2H4	5.40E+17	-1.45	26040	REV/1.0E11 0.0E0 1.06E4/
2467	NC3H7COC2H4S=CH3CHCO+NC3H7	1.97E+19	-1.49	42860	REV/2.719E11 2.9E-1 3.62E4/
2468	CHCHCHO+OH=CH2CHO+HCO	1.00E+12	0	0	
2469	O2+C6H12-1=>CH2O+NC4H9CHO	1.00E+14	0	37000	
2470	C6H12-1=2C3H6	4.00E+12	0	58000	
2471	C6H111-3+H=C6H12-1	1.00E+14	0	0	
2472	C5H91-5+CH3=C6H12-1	1.00E+13	0	0	
2473	PC4H9+C2H3=C6H12-1	1.00E+13	0	0	

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Table B .1. (cont.)

2474	C4H71-4+C2H5=C6H12-1	8.00E+12	0	0	
2475	C6H111-3+H=C6H12-2	1.00E+14	0	0	
2476	C6H112-4+H=C6H12-2	1.00E+14	0	0	
2477	C5H92-5+CH3=C6H12-2	1.00E+13	0	0	
2478	NC3H7+C3H5-T=C6H12-2	1.00E+13	0	0	
2479	C6H112-4+H=C6H12-3	1.00E+14	0	0	
2480	C4H71-1+C2H5=C6H12-3	1.00E+13	0	0	
2481	C6H12-1+O2=C6H111-3+HO2	2.20E+12	0	37220	
2482	C6H12-1+O2=C6H111-4+HO2	2.00E+13	0	49640	
2483	C6H12-1+O2=C6H111-5+HO2	2.00E+13	0	49640	
2484	C6H12-1+O2=C6H111-6+HO2	3.00E+13	0	52290	
2485	C6H12-1+O=C6H111-3+OH	6.60E+05	2.43	1210	
2486	C6H12-1+O=C6H111-4+OH	5.51E+05	2.45	2830	
2487	C6H12-1+O=C6H111-5+OH	5.51E+05	2.45	2830	
2488	C6H12-1+O=C6H111-6+OH	9.80E+05	2.43	4750	
2489	C6H12-2+O2=C6H111-3+HO2	5.50E+12	0	39900	
2490	C6H12-2+O2=C6H112-4+HO2	2.20E+12	0	37220	
2491	C6H12-2+O2=C6H112-5+HO2	2.00E+13	0	49640	
2492	C6H12-2+O2=C6H112-6+HO2	3.00E+13	0	52290	
2493	C6H12-2+O=C6H111-3+OH	4.41E+05	2.42	3150	
2494	C6H12-2+O=C6H112-4+OH	6.60E+05	2.43	1210	
2495	C6H12-2+O=C6H112-5+OH	5.51E+05	2.45	2830	
2496	C6H12-2+O=C6H112-6+OH	9.80E+05	2.43	4750	
2497	C6H12-3+O2=C6H112-4+HO2	4.40E+12	0	37220	
2498	C6H12-3+O2=C6H113-1+HO2	6.00E+13	0	52290	
2499	C6H12-3+O=C6H112-4+OH	1.32E+06	2.43	1210	
2500	C6H12-3+O=C6H113-1+OH	1.96E+06	2.43	4750	
2501	C2H5+C4H6=C6H111-3	8.50E+10	0	8300	
2502	CH3+C5H81-4=C6H111-4	1.00E+11	0	7800	
2503	C3H5-A+C3H6=C6H111-5	4.00E+11	0	16900	
2504	C4H71-4+C2H4=C6H111-6	1.00E+11	0	8200	
2505	CH3+C5H81-3=C6H112-4	6.00E+10	0	7500	
2506	C3H5-T+C3H6=C6H112-5	6.30E+11	0	3100	
2507	C4H71-3+C2H4=C6H112-6	4.00E+11	0	13050	
2508	C4H71-1+C2H4=C6H113-1	6.30E+11	0	3100	
2509	C6H111-6=C6H111-4	3.80E+10	0.67	36000	
2510	C6H111-6=C6H111-5	3.56E+10	0.88	37300	
2511	C6H112-6=C6H112-4	3.80E+10	0.67	28400	
2512	C6H112-6=C6H112-5	3.56E+10	0.88	37300	
2513	C6H113-1=C6H112-4	3.56E+10	0.88	29600	
2514	C6H111-3+O2=C6H112O2-1	2.00E+12	0	0	
2515	C6H111-3+O2=C6H111O2-3	2.00E+12	0	0	
2516	C6H111-4+O2=C6H111O2-4	7.54E+12	0	0	
2517	C6H111-5+O2=C6H111O2-5	7.54E+12	0	0	
2518	C6H111-6+O2=C6H111O2-6	4.52E+12	0	0	
2519	C6H112-4+O2=C6H113O2-2	2.00E+12	0	0	
2520	C6H112-4+O2=C6H112O2-4	2.00E+12	0	0	
2521	C6H112-5+O2=C6H112O2-5	7.54E+12	0	0	

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Table B .1. (cont.)

2522	C6H112-6+O2=C6H112O2-6	4.52E+12	0	0	
2523	C6H113-1+O2=C6H113O2-1	4.52E+12	0	0	
2524	C6H111O2-3=>C6H101-3+HO2	1.00E+39	-8.11	40500	
2525	C6H111O2-4=>C6H101-3+HO2	2.04E+38	-8.11	38500	
2526	C6H111O2-5=>C6H101-4+HO2	1.00E+39	-8.11	40500	
2527	C6H111O2-6=>C6H101-5+HO2	1.00E+39	-8.11	40500	
2528	C6H111O2-5=>C6H101-5+HO2	1.01E+43	-9.41	41500	
2529	C6H112O2-4=>C6H101-3+HO2	5.04E+38	-8.11	40500	
2530	C6H112O2-5=>C6H102-4+HO2	1.04E+38	-8.11	37500	
2531	C6H112O2-6=>C6H101-4+HO2	5.04E+38	-8.11	40500	
2532	C6H113O2-2=>C6H101-3+HO2	5.08E+42	-9.41	41500	
2533	C6H113O2-1=>C6H101-3+HO2	1.04E+38	-8.11	37500	
2534	C6H111O2-3=C6H101OOH3-4	2.00E+11	0	26450	
2535	C6H111O2-3=C6H101OOH3-5	2.50E+10	0	20450	
2536	C6H111O2-3=C6H101OOH3-6	9.38E+09	0	21950	
2537	C6H111O2-4=C6H101OOH4-3	2.00E+11	0	24450	
2538	C6H111O2-4=C6H101OOH4-5	2.00E+11	0	26450	
2539	C6H111O2-4=C6H101OOH4-6	3.75E+10	0	24000	
2540	C6H111O2-5=C6H101OOH5-3	2.50E+10	0	18450	
2541	C6H111O2-5=C6H101OOH5-4	2.00E+11	0	26450	
2542	C6H111O2-5=C6H101OOH5-6	3.00E+11	0	29000	
2543	C6H111O2-6=C6H101OOH6-3	3.13E+09	0	16650	
2544	C6H111O2-6=C6H101OOH6-4	2.50E+10	0	20450	
2545	C6H111O2-6=C6H101OOH6-5	2.00E+11	0	26450	
2546	C6H112O2-4=C6H102OOH4-5	2.00E+11	0	26450	
2547	C6H112O2-4=C6H102OOH4-6	3.75E+10	0	24000	
2548	C6H112O2-5=C6H102OOH5-4	2.00E+11	0	24450	
2549	C6H112O2-5=C6H102OOH5-6	3.00E+11	0	29000	
2550	C6H112O2-6=C6H102OOH6-4	2.50E+10	0	18450	
2551	C6H112O2-6=C6H102OOH6-5	2.00E+11	0	26450	
2552	C6H113O2-1=C6H103OOH1-2	2.00E+11	0	24450	
2553	C6H113O2-2=C6H103OOH2-1	3.00E+11	0	29000	
2554	C6H101OOH3-4=>ETES1+OH	6.00E+11	0	22000	
2555	C6H101OOH3-5=>MVOX+OH	7.50E+10	0	15250	
2556	C6H101OOH3-4=>VTHF+OH	9.38E+09	0	7000	
2557	C6H101OOH4-3=>EDHF+OH	9.38E+09	0	7000	
2558	C6H101OOH4-3=>ETES1+OH	6.00E+11	0	22000	
2559	C6H101OOH4-5=>ETES1+OH	6.00E+11	0	22000	
2560	C6H101OOH4-6=>ETES1+OH	7.50E+10	0	15250	
2561	C6H101OOH5-3=>MVOX+OH	7.50E+10	0	15250	
2562	C6H101OOH5-4=>ETES1+OH	6.00E+11	0	22000	
2563	C6H101OOH5-6=>ETES1+OH	6.00E+11	0	22000	
2564	C6H101OOH6-3=>VTHF+OH	9.38E+09	0	7000	
2565	C6H101OOH6-4=>ETES1+OH	7.50E+10	0	15250	
2566	C6H101OOH6-5=>ETES1+OH	6.00E+11	0	22000	
2567	C6H102OOH4-5=>ETES1+OH	6.00E+11	0	22000	
2568	C6H102OOH4-6=>ETES1+OH	7.50E+10	0	15250	
2569	C6H102OOH5-4=>ETES1+OH	6.00E+11	0	22000	

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Table B .1. (cont.)

2570	C6H102OOH5-6=>ETES1+OH	6.00E+11	0	22000	
2571	C6H102OOH6-4=>ETES1+OH	7.50E+10	0	15250	
2572	C6H102OOH6-5=>ETES1+OH	6.00E+11	0	22000	
2573	C6H103OOH2-1=>ETES1+OH	6.00E+11	0	22000	
2574	C6H103OOH1-2=>ETES1+OH	6.00E+11	0	22000	
2575	HO2+C6H101-3=C6H101OOH3-4	4.85E+11	0	10000	
2576	HO2+C6H101-3=C6H101OOH4-3	4.85E+11	0	9000	
2577	HO2+C6H101-4=C6H101OOH4-5	3.40E+11	0	11800	
2578	HO2+C6H101-4=C6H101OOH5-4	3.40E+11	0	11800	
2579	HO2+C6H101-5=C6H101OOH5-6	1.00E+12	0	13700	
2580	HO2+C6H101-5=C6H101OOH6-5	1.00E+12	0	13700	
2581	HO2+C6H102-4=C6H102OOH4-5	3.80E+11	0	8800	
2582	HO2+C6H102-4=C6H102OOH5-4	3.80E+11	0	7800	
2583	HO2+C6H101-4=C6H102OOH5-6	1.00E+12	0	13700	
2584	HO2+C6H101-4=C6H102OOH6-5	1.00E+12	0	13700	
2585	HO2+C6H101-3=C6H103OOH2-1	4.85E+11	0	10000	
2586	HO2+C6H101-3=C6H103OOH1-2	4.85E+11	0	9000	
2587	C6H12-1+HO2=C6H12OOH1-2	1.00E+12	0	13700	
2588	C6H12-1+HO2=C6H12OOH2-1	1.00E+12	0	13700	
2589	C6H12-2+HO2=C6H12OOH2-3	6.80E+11	0	11800	
2590	C6H12-2+HO2=C6H12OOH3-2	6.80E+11	0	11800	
2591	C6H12-3+HO2=C6H12OOH3-4	6.80E+11	0	11800	
2592	C6H101OOH3-4=>CH3+AC3H5OOH+C2H2	3.00E+13	0	33500	
2593	C6H101OOH3-5=>OH+C3H6+C2H3CHO	3.00E+13	0	23000	
2594	C6H101OOH3-6=>HO2+C4H6+C2H4	3.00E+13	0	30000	
2595	C6H101OOH4-3=>C2H5+CH3O2H+C3H2	1.00E+13	0	35000	
2596	C6H101OOH4-5=>C3H5-A+AC3H5OOH	3.00E+13	0	23000	
2597	C6H101OOH4-6=>OH+C2H3COCH3+C2H4	3.00E+13	0	30000	
2598	C6H101OOH5-3=>OH+C4H6+CH3CHO	1.00E+13	0	35000	
2599	C6H101OOH5-4=>CH3+CH3O2H+2C2H2	3.00E+13	0	33500	
2600	C6H101OOH5-6=>C4H71-4+C2H3OOH	3.00E+13	0	30000	
2601	C6H101OOH6-3=>HO2+C4H6+C2H4	1.00E+13	0	35000	
2602	C6H101OOH6-4=>OH+C5H81-4+CH2O	3.00E+13	0	29500	
2603	C6H101OOH6-5=>C3H5-A+AC3H5OOH	3.00E+13	0	23000	
2604	C6H102OOH4-6=>OH+C2H3COCH3+C2H4	3.00E+13	0	22000	
2605	C6H102OOH5-6=>C4H71-3+CH2CHO+OH	3.00E+13	0	22000	
2606	C6H102OOH6-4=>OH+C5H81-3+CH2O	1.00E+13	0	35000	
2607	C6H102OOH6-5=>C3H5-T+AC3H5OOH	3.00E+13	0	39000	
2608	C6H103OOH2-1=>C4H71-4+CH2CHO+OH	3.00E+13	0	39000	
2609	C6H101OOH3-4+O2=C6H101OOH3-4O2	7.54E+12	0	0	
2610	C6H101OOH3-5+O2=C6H101OOH3-5O2	7.54E+12	0	0	
2611	C6H101OOH3-6+O2=C6H101OOH3-6O2	4.52E+12	0	0	
2612	C6H101OOH4-3+O2=C6H101OOH4-3O2	2.00E+12	0	0	
2613	C6H101OOH4-5+O2=C6H101OOH4-5O2	7.54E+12	0	0	
2614	C6H101OOH4-6+O2=C6H101OOH4-6O2	4.52E+12	0	0	
2615	C6H101OOH5-3+O2=C6H101OOH5-3O2	2.00E+12	0	0	
2616	C6H101OOH5-4+O2=C6H101OOH5-4O2	7.54E+12	0	0	
2617	C6H101OOH5-6+O2=C6H101OOH5-6O2	4.52E+12	0	0	

(cont. on next page)

Table B .1. (cont.)

2618	C6H101OOH6-3+O2=C6H101OOH6-3O2	2.00E+12	0	0	
2619	C6H101OOH6-4+O2=C6H101OOH6-4O2	7.54E+12	0	0	
2620	C6H101OOH6-5+O2=C6H101OOH6-5O2	7.54E+12	0	0	
2621	C6H102OOH4-5+O2=C6H102OOH4-5O2	7.54E+12	0	0	
2622	C6H102OOH4-6+O2=C6H102OOH4-6O2	4.52E+12	0	0	
2623	C6H102OOH5-4+O2=C6H102OOH5-4O2	1.00E+12	0	0	
2624	C6H102OOH5-6+O2=C6H102OOH5-6O2	4.52E+12	0	0	
2625	C6H102OOH6-4+O2=C6H102OOH6-4O2	1.00E+12	0	0	
2626	C6H102OOH6-5+O2=C6H102OOH6-5O2	7.54E+12	0	0	
2627	C6H103OOH2-1+O2=C6H103OOH2-1O2	4.52E+12	0	0	
2628	C6H103OOH1-2+O2=C6H103OOH1-2O2	1.00E+12	0	0	
2629	C6H101OOH3-4O2=>NC6D1KET34+OH	1.00E+11	0	21450	
2630	C6H101OOH3-5O2=>NC6D1KET35+OH	1.25E+10	0	15450	
2631	C6H101OOH3-6O2=>NC6D1KET36+OH	1.56E+09	0	13650	
2632	C6H101OOH4-3O2=>NC6D1KET43+OH	1.00E+11	0	23450	
2633	C6H101OOH4-5O2=>NC6D1KET45+OH	1.00E+11	0	23450	
2634	C6H101OOH4-6O2=>NC6D1KET46+OH	1.25E+10	0	17450	
2635	C6H101OOH5-3O2=>NC6D1KET53+OH	1.25E+10	0	17450	
2636	C6H101OOH5-4O2=>NC6D1KET54+OH	1.00E+11	0	23450	
2637	C6H101OOH5-6O2=>NC6D1KET56+OH	1.00E+11	0	23450	
2638	C6H101OOH6-3O2=>NC6D1KET63+OH	3.12E+09	0	22150	
2639	C6H101OOH6-4O2=>NC6D1KET64+OH	2.50E+10	0	21000	
2640	C6H101OOH6-5O2=>NC6D1KET65+OH	2.00E+11	0	26150	
2641	C6H102OOH4-5O2=>NC6D2KET45+OH	1.00E+11	0	21450	
2642	C6H102OOH4-6O2=>NC6D2KET46+OH	1.25E+10	0	15450	
2643	C6H102OOH5-4O2=>NC6D2KET54+OH	1.00E+11	0	23450	
2644	C6H102OOH5-6O2=>NC6D2KET56+OH	1.00E+11	0	23450	
2645	C6H102OOH6-4O2=>NC6D2KET64+OH	2.50E+10	0	21000	
2646	C6H102OOH6-5O2=>NC6D2KET65+OH	2.00E+11	0	26000	
2647	C6H103OOH2-1O2=>NC6D3KET21+OH	1.00E+11	0	21450	
2648	C6H103OOH1-2O2=>NC6D3KET12+OH	2.00E+11	0	26000	
2649	NC6D1KET34=>OH+C2H3+CO+C2H5CHO	1.00E+16	0	39000	
2650	NC6D1KET35=>OH+CH2CHO+C2H3COCH3	5.00E+15	0	39000	
2651	NC6D1KET35=>OH+CH3+CO+C2H3COCH3	5.00E+15	0	39000	
2652	NC6D1KET36=>OH+C2H3+CO+CH2O+C2H4	1.00E+16	0	39000	
2653	NC6D1KET43=>OH+C3H5O+C2H3CHO	1.00E+16	0	39000	
2654	NC6D1KET45=>OH+C2H3+CH3CHO+CH2CO	1.00E+16	0	39000	
2655	NC6D1KET46=>OH+C3H5-A+CO+CH3CHO	1.00E+16	0	39000	
2656	NC6D1KET53=>OH+C2H5CO+C2H3CHO	1.00E+16	0	39000	
2657	NC6D1KET54=>OH+C3H5-A+CO+CH3CHO	1.00E+16	0	39000	
2658	NC6D1KET56=>OH+C3H5-A+CH2CO+CH2O	1.00E+16	0	39000	
2659	NC6D1KET63=>OH+C2H3CHO+HCO+C2H4	1.00E+16	0	39000	
2660	NC6D1KET64=>OH+C3H5-A+CH3CHO+CO	5.00E+15	0	39000	
2661	NC6D1KET64=>OH+CH2CHO+AC3H5CHO	5.00E+15	0	39000	
2662	NC6D1KET65=>OH+HCO+CH2CO+C3H6	1.00E+16	0	39000	
2663	NC6D2KET45=>OH+C3H5-T+CO+CH3CHO	1.00E+16	0	39000	
2664	NC6D2KET46=>OH+C3H5-T+CH2CO+CH2O	1.00E+16	0	39000	
2665	NC6D2KET54=>OH+CH2CHO+C2H3COCH3	1.00E+16	0	39000	

(cont. on next page)

Table B .1. (cont.)

2666	NC6D2KET56=>OH+C3H5-T+CH2O+CH2CO	1.00E+16	0	39000	
2667	NC6D2KET64=>OH+CH2CHO+C2H3COCH3	1.00E+16	0	39000	
2668	NC6D2KET65=>OH+C4H71-3+CO+CH2O	1.00E+16	0	39000	
2669	NC6D3KET21=>OH+C4H71-4+CO+CH2O	1.00E+16	0	39000	
2670	NC6D3KET12=>OH+HCO+C4H7CHO1-4	1.00E+16	0	39000	
2671	C6H12OH-1=>CH3CHO+PC4H9	1.50E+13	0	30000	
2672	C6H12OH-1=>C2H5CHO+NC3H7	1.50E+13	0	30000	
2673	C6H12OH-2=>NC3H7CHO+C2H5	1.50E+13	0	30000	
2674	C6H12OH-2=>NC4H9CHO+CH3	1.50E+13	0	30000	
2675	C6H12OH-3=>NC3H7CHO+C2H5	3.00E+13	0	30000	
2676	C6H12-3+O=NC3H7+C2H5CO	1.00E+11	0	-1050	
2677	C6H111-4+HO2=C6H111O2H-4	9.00E+12	0	0	
2678	C6H111-5+HO2=C6H111O2H-5	9.00E+12	0	0	
2679	C6H111-6+HO2=C6H111O2H-6	9.00E+12	0	0	
2680	C6H112-5+HO2=C6H112O2H-5	9.00E+12	0	0	
2681	C6H112-6+HO2=C6H112O2H-6	9.00E+12	0	0	
2682	C6H112-4+HO2=C6H113O2H-2	4.00E+12	0	0	
2683	C6H112-4+HO2=C6H112O2H-4	4.00E+12	0	0	
2684	C6H113-1+HO2=C6H113O2H-1	9.00E+12	0	0	
2685	C6H112O2-1=>C2H3COC3H7+OH	4.00E+12	0	38000	
2686	C6H111O2-3=>C2H3COC3H7+OH	4.00E+12	0	38000	
2687	C6H101OOH3-6=>C2H3COC3H7+OH	1.00E+11	0	16700	
2688	C6H111O2H-4=>OH+C2H5CHO+C3H5-A	1.00E+16	0	39000	
2689	C6H111O2H-5=>OH+CH3CHO+C4H71-4	1.00E+16	0	39000	
2690	C6H111O2H-6=>OH+CH2O+C5H91-5	1.00E+16	0	39000	
2691	C6H112O2H-4=>OH+C2H3COCH3+C2H5	1.00E+16	0	39000	
2692	C6H112O2H-5=>OH+CH3CHO+C4H71-3	1.00E+16	0	39000	
2693	C6H112O2H-6=>OH+CH2O+C5H91-5	1.00E+16	0	39000	
2694	C6H113O2H-2=>OH+CH3CHO+C4H71-4	1.00E+16	0	39000	
2695	C6H113O2H-1=>OH+CH2O+C5H91-3	1.00E+16	0	39000	
2696	O2+ETES1=>HO2+C2H3COCH3+C2H3	2.05E+07	2	40722.49	
2697	H+ETES1=>H2+C2H3COCH3+C2H3	2.57E+07	2	3950.57	
2698	OH+ETES1=>H2O+C2H3COCH3+C2H3	4.79E+06	2	-2259.83	
2699	O+ETES1=>OH+C2H3COCH3+C2H3	1.62E+07	2	2579.54	
2700	HO2+ETES1=>H2O2+C2H3COCH3+C2H3	6.47E+05	2	11887.73	
2701	HCO+ETES1=>CH2O+C2H3COCH3+C2H3	1.52E+06	2	12360.44	
2702	CH3+ETES1=>CH4+C2H3COCH3+C2H3	4.68E+05	2	4871.29	
2703	C2H5+ETES1=>C2H6+C2H3COCH3+C2H3	2.76E+05	2	7658.07	
2704	CH3O+ETES1=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2	1583.56	
2705	CH3O2+ETES1=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2	12360.44	
2706	O2+MVOX=>HO2+C2H3COCH3+C2H3	2.05E+07	2	40722.49	
2707	H+MVOX=>H2+C2H3COCH3+C2H3	2.57E+07	2	3950.57	
2708	OH+MVOX=>H2O+C2H3COCH3+C2H3	4.79E+06	2	-2259.83	
2709	O+MVOX=>OH+C2H3COCH3+C2H3	1.62E+07	2	2579.54	
2710	HO2+MVOX=>H2O2+C2H3COCH3+C2H3	6.47E+05	2	11887.73	
2711	HCO+MVOX=>CH2O+C2H3COCH3+C2H3	1.52E+06	2	12360.44	
2712	CH3+MVOX=>CH4+C2H3COCH3+C2H3	4.68E+05	2	4871.29	
2713	C2H5+MVOX=>C2H6+C2H3COCH3+C2H3	2.76E+05	2	7658.07	

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Table B .1. (cont.)

2714	CH3O2+MVOX=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2	12360.44	
2715	C2H3+MVOX=>C2H4+C2H3COCH3+C2H3	8.14E+05	2	4871.29	
2716	CH3O+MVOX=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2	1583.56	
2717	O2+VTHF=>HO2+C2H3COCH3+C2H3	2.05E+07	2	40722.49	
2718	H+VTHF=>H2+C2H3COCH3+C2H3	2.57E+07	2	3950.57	
2719	OH+VTHF=>H2O+C2H3COCH3+C2H3	4.79E+06	2	-2259.83	
2720	O+VTHF=>OH+C2H3COCH3+C2H3	1.62E+07	2	2579.54	
2721	HO2+VTHF=>H2O2+C2H3COCH3+C2H3	6.47E+05	2	11887.73	
2722	HCO+VTHF=>CH2O+C2H3COCH3+C2H3	1.52E+06	2	12360.44	
2723	CH3+VTHF=>CH4+C2H3COCH3+C2H3	4.68E+05	2	4871.29	
2724	C2H5+VTHF=>C2H6+C2H3COCH3+C2H3	2.76E+05	2	7658.07	
2725	CH3O+VTHF=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2	1583.56	
2726	CH3O2+VTHF=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2	12360.44	
2727	C2H3+VTHF=>C2H4+C2H3COCH3+C2H3	8.14E+05	2	4871.29	
2728	O2+EDHF=>HO2+C2H3COCH3+C2H3	2.05E+07	2	40722.49	
2729	H+EDHF=>H2+C2H3COCH3+C2H3	2.57E+07	2	3950.57	
2730	OH+EDHF=>H2O+C2H3COCH3+C2H3	4.79E+06	2	-2259.83	
2731	O+EDHF=>OH+C2H3COCH3+C2H3	1.62E+07	2	2579.54	
2732	HO2+EDHF=>H2O2+C2H3COCH3+C2H3	6.47E+05	2	11887.73	
2733	HCO+EDHF=>CH2O+C2H3COCH3+C2H3	1.52E+06	2	12360.44	
2734	CH3+EDHF=>CH4+C2H3COCH3+C2H3	4.68E+05	2	4871.29	
2735	C2H5+EDHF=>C2H6+C2H3COCH3+C2H3	2.76E+05	2	7658.07	
2736	C2H3+EDHF=>C2H4+C2H3COCH3+C2H3	8.14E+05	2	4871.29	
2737	CH3O2+EDHF=>CH3O2H+C2H3COCH3+C2H3	9.13E+05	2	12360.44	
2738	CH3O+EDHF=>CH3OH+C2H3COCH3+C2H3	5.14E+05	2	1583.56	
2739	O2+C5H81-4=>HO2+C3H5-A+C2H2	5.11E+06	2	40722.49	
2740	H+C5H81-4=>H2+C3H5-A+C2H2	6.44E+06	2	3950.57	
2741	OH+C5H81-4=>H2O+C3H5-A+C2H2	1.20E+06	2	-2259.83	
2742	O+C5H81-4=>OH+C3H5-A+C2H2	4.06E+06	2	2579.54	
2743	HO2+C5H81-4=>H2O2+C3H5-A+C2H2	1.62E+05	2	11887.73	
2744	HCO+C5H81-4=>CH2O+C3H5-A+C2H2	3.79E+05	2	12360.44	
2745	CH3+C5H81-4=>CH4+C3H5-A+C2H2	1.17E+05	2	4871.29	
2746	C2H5+C5H81-4=>C2H6+C3H5-A+C2H2	6.90E+04	2	7658.07	
2747	CH3O+C5H81-4=>CH3OH+C3H5-A+C2H2	1.28E+05	2	1583.56	
2748	CH3O2+C5H81-4=>CH3O2H+C3H5-A+C2H2	2.28E+05	2	12360.44	
2749	C2H3+C5H81-4=>C2H4+C3H5-A+C2H2	2.04E+05	2	4871.29	
2750	C6H101-3+H=C6H111-3	2.50E+11	0.5	2620	
2751	C6H101-3+H=C6H111-4	2.50E+11	0.5	2620	
2752	C6H101-3+H=C6H113-1	4.25E+11	0.5	1230	
2753	C6H101-3+H=C6H112-4	2.50E+11	0.5	2620	
2754	C6H101-4+H=C6H111-4	2.50E+11	0.5	2620	
2755	C6H101-4+H=C6H111-5	2.50E+11	0.5	2620	
2756	C6H101-4+H=C6H112-5	4.25E+11	0.5	1230	
2757	C6H101-4+H=C6H112-6	2.50E+11	0.5	2620	
2758	C6H101-5+H=C6H111-5	4.25E+11	0.5	1230	
2759	C6H101-5+H=C6H111-6	2.50E+11	0.5	2620	
2760	C6H101-3+O=>C5H91-3+HCO	2.00E+11	0	-1050	
2761	C6H101-4+O=>C5H92-5+HCO	2.00E+11	0	-1050	

(cont. on next page)

Table B .1. (cont.)

2762	C6H101-5+O=>C5H91-5+HCO	2.00E+11	0	-1050	
2763	C6H101-3+OH=>C5H91-3+CH2O	1.00E+12	0	0	
2764	C6H101-4+OH=>C5H92-5+CH2O	1.00E+12	0	0	
2765	C6H101-5+OH=>C5H91-5+CH2O	1.00E+12	0	0	
2766	C6H101-3+OH=>C2H3+C4H6+H2O	2.76E+04	2.64	-1919	
2767	C6H101-4+OH=>C2H3+C4H6+H2O	2.76E+04	2.64	-1919	
2768	C6H101-5+OH=>C2H3+C4H6+H2O	2.76E+04	2.64	-1919	
2769	C6H101-3+HO2=>C2H3+C4H6+H2O2	4.82E+03	2.55	10530	
2770	C6H101-4+HO2=>C2H3+C4H6+H2O2	4.82E+03	2.55	10530	
2771	C6H101-5+HO2=>C2H3+C4H6+H2O2	4.82E+03	2.55	10530	
2772	C6H101-3+H=>C2H3+C4H6+H2	3.38E+05	2.36	207	
2773	C6H101-4+H=>C2H3+C4H6+H2	3.38E+05	2.36	207	
2774	C6H101-5+H=>C2H3+C4H6+H2	3.38E+05	2.36	207	
2775	2OH=O+H2O	3.57E+04	2.4	-2110	
2776	2H+M=H2+M	1.00E+18	-1	0	Third body: AR /0.63/ Third body: C2H6 /3.0/ Third body: H2O /0.0/ Third body: CO2 /0.0/ Third body: H2 /0.0/ Third body: CH4 /2.0/
2777	2H+H2=2H2	9.00E+16	-0.6	0	
2778	2H+H2O=H2+H2O	6.00E+19	-1.25	0	
2779	2H+CO2=H2+CO2	5.50E+20	-2	0	
2780	H+OH+M=H2O+M	2.20E+22	-2	0	Third body: AR /0.38/ Third body: C2H6 /3.0/ Third body: H2O /3.65/ Third body: H2 /0.73/ Third body: CH4 /2.0/
2781	H+2O2=HO2+O2	3.00E+20	-1.72	0	
2782	H+O2+H2O=HO2+H2O	9.38E+18	-0.76	0	
2783	H+O2+N2=HO2+N2	3.75E+20	-1.72	0	
2784	H+O2+AR=HO2+AR	7.00E+17	-0.8	0	
2785	HO2+H=O+H2O	3.97E+12	0	671	
2786	H2O2+H=OH+H2O	1.00E+13	0	3600	
2787	CO+O2=CO2+O	2.50E+12	0	47800	
2788	CH+H=C+H2	1.10E+14	0	0	
2789	CH+CO(+M)=HCCO(+M)	5.00E+13	0	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.69E28 -3.74E0 1.936E3/ TROE/5.757E-1 2.37E2 1.652E3 5.069E3/
2790	CH+CO2=HCO+CO	3.40E+12	0	690	
2791	CH2+O=HCO+H	8.00E+13	0	0	
2792	CH2+OH=CH2O+H	2.00E+13	0	0	
2793	CH2+HO2=CH2O+OH	2.00E+13	0	0	
2794	CH2+C=C2H+H	5.00E+13	0	0	
2795	CH2+CH=C2H2+H	4.00E+13	0	0	
2796	2CH2=C2H2+H2	3.20E+13	0	0	
2797	CH2(S)+N2=CH2+N2	1.50E+13	0	600	
2798	CH2(S)+AR=CH2+AR	9.00E+12	0	600	

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Table B .1. (cont.)

2799	CH2(S)+O=CO+H2	1.50E+13	0	0	
2800	CH2(S)+O=HCO+H	1.50E+13	0	0	
2801	CH2(S)+O2=CO+H2O	1.20E+13	0	0	
2802	CH2(S)+H2O(+M)=CH3OH(+M)	2.00E+13	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.7E38 -6.3E0 3.1E3/ TROE/1.507E-1 1.34E2 2.383E3 7.265E3/
2803	CH2(S)+CO=CH2+CO	9.00E+12	0	0	
2804	CH2(S)+CO2=CH2+CO2	7.00E+12	0	0	
2805	CH2(S)+CO2=CH2O+CO	1.40E+13	0	0	
2806	CH2O+HO2=HCO+H2O2	1.00E+12	0	8000	
2807	CH3+C=C2H2+H	5.00E+13	0	0	
2808	CH3+CH=C2H3+H	3.00E+13	0	0	
2809	CH3+CH2O=CH4+HCO	3.32E+03	2.81	5860	
2810	CH3+CH2=C2H4+H	4.00E+13	0	0	
2811	CH3O+H(+M)=CH3OH(+M)	5.00E+13	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/8.6E28 -4.0E0 3.025E3/ TROE/8.902E-1 1.44E2 2.838E3 4.5569E4/
2812	CH3O+H=CH2OH+H	3.40E+06	1.6	0	
2813	CH3O+H=CH2O+H2	2.00E+13	0	0	
2814	CH3O+H=CH2(S)+H2O	1.60E+13	0	0	
2815	CH3O+O=CH2O+OH	1.00E+13	0	0	
2816	CH3O+OH=CH2O+H2O	5.00E+12	0	0	
2817	CH2OH+H=CH2O+H2	2.00E+13	0	0	
2818	CH2OH+H=CH2(S)+H2O	6.00E+12	0	0	
2819	CH2OH+O=CH2O+OH	1.00E+13	0	0	
2820	CH2OH+OH=CH2O+H2O	5.00E+12	0	0	
2821	CH3OH+H=CH3O+H2	4.20E+06	2.1	4870	
2822	CH3OH+O=CH3O+OH	1.30E+05	2.5	5000	
2823	CH3OH+OH=CH3O+H2O	6.30E+06	2	1500	
2824	C2H+O=CH+CO	5.00E+13	0	0	
2825	C2H+OH=H+HCCO	2.00E+13	0	0	
2826	C2H+O2=HCO+CO	5.00E+13	0	1500	
2827	C2H+H2=H+C2H2	4.90E+05	2.5	560	
2828	HCCO+O2=OH+2CO	1.60E+12	0	854	
2829	HCCO+CH2=C2H3+CO	3.00E+13	0	0	
2830	2HCCO=C2H2+2CO	1.00E+13	0	0	
2831	C2H2+O=CH2+CO	3.50E+03	2.8	500	

(cont. on next page)

Table B .1. (cont.)

2832	C2H3+H(+M)=C2H4(+M)	6.08E+12	0.27	280	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/1.4E30 -3.86E0 3.32E3/ TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
2833	C2H3+O=CH2CO+H	3.00E+13	0	0	
2834	C2H3+O2=C2H2+HO2	1.66E+14	-0.83	2540	
2835	C2H3+O2=CH2CHO+O	3.50E+14	-0.611	5260	
2836	C2H4+H=C2H3+H2	1.33E+06	2.53	12240	
2837	C2H4+O=CH3+HCO	1.92E+07	1.83	220	
2838	C2H4+OH=C2H3+H2O	3.60E+06	2	2500	
2839	C2H5+O=CH3+CH2O	1.32E+14	0	0	
2840	C2H5+O2=C2H4+HO2	8.40E+11	0	3875	
2841	C2H6+CH2*=C2H5+CH3	4.00E+13	0	-550	
2842	HCCO+OH=C2O+H2O	3.00E+13	0	0	
2843	C2O+H=CH+CO	5.00E+13	0	0	
2844	C2O+O=2CO	5.00E+13	0	0	
2845	C2O+OH=2CO+H	2.00E+13	0	0	
2846	C2O+O2=2CO+O	2.00E+13	0	0	
2847	CH2CO+H=CH2CHO	5.40E+11	0.454	1820	
2848	CH2CHO+O=CH2O+HCO	9.60E+06	1.83	220	
2849	CH2CHO+O=CH2CO+OH	1.00E+13	0	0	
2850	CH2CHO+OH=CH2CO+H2O	5.00E+12	0	0	
2851	CH3+HCCO=C2H4+CO	5.00E+13	0	0	
2852	CH3+C2H=C3H3+H	2.41E+13	0	0	
2853	CH4+C2H=C2H2+CH3	1.81E+12	0	500	
2854	C2H2+CH=C3H2+H	3.00E+13	0	0	
2855	C2H2+CH2=C3H3+H	1.20E+13	0	6620	
2856	C2H2+CH2*=C3H3+H	2.00E+13	0	0	
2857	C2H2+CH3=C3H4-P+H	2.72E+18	-1.97	20200	
2858	C2H+C2H2=H+C4H2	3.00E+14	0	0	
2859	C2H2+C2H=n-C4H3	4.50E+37	-7.68	7100	
2860	C2H2+C2H=i-C4H3	2.60E+44	-9.47	14650	
2861	C2H2+C2H3=C4H4+H	2.00E+18	-1.68	10600	
2862	C2H2+C2H3=C4H5-N	9.30E+38	-8.76	12000	
2863	C2H2+C2H3=C4H5-I	1.60E+46	-10.98	18600	
2864	C2H4+C2H=C4H4+H	1.20E+13	0	0	
2865	C2H4+C2H3=C4H6+H	2.80E+21	-2.44	14720	
2866	C2H4+O2=C2H3+HO2	4.22E+13	0	60800	
2867	C2H3+H2O2=C2H4+HO2	1.21E+10	0	-596	
2868	C2H3+HCO=C2H4+CO	2.50E+13	0	0	
2869	2C2H3=C4H6	1.50E+42	-8.84	12483	
2870	2C2H3=C4H5-N+H	2.40E+20	-2.04	15361	
2871	C3H2+O=C2H2+CO	6.80E+13	0	0	
2872	C3H2+CH=C4H2+H	5.00E+13	0	0	
2873	C3H2+CH2=n-C4H3+H	5.00E+13	0	0	
2874	C3H2+CH3=C4H4+H	5.00E+12	0	0	

(cont. on next page)

Table B .1. (cont.)

2875	C3H2+HCCO=n-C4H3+CO	1.00E+13	0	0	
2876	C3H3+OH=C2H3+HCO	4.00E+13	0	0	
2877	C3H3+HCO=C3H4-A+CO	2.50E+13	0	0	
2878	C3H3+HCO=C3H4-P+CO	2.50E+13	0	0	
2879	C3H3+CH=i-C4H3+H	5.00E+13	0	0	
2880	C3H3+CH3(+M)=C4H612(+M)	1.50E+13	0	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.6E58 -1.194E1 9.77E3/ TROE/1.75E-1 1.3406E3 6.0E4 9.7698E3/
2881	C3H4-A+H=C3H3+H2	6.63E+03	3.095	5522	
2882	C3H4-A+O=CH2CO+CH2	2.00E+07	1.8	1000	
2883	C3H4-A+OH=C3H3+H2O	5.30E+06	2	2000	
2884	C4H+H(+M)=C4H2(+M)	1.00E+17	-1	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.75E33 -4.8E0 1.9E3/ TROE/6.464E-1 1.32E2 1.315E3 5.566E3/
2885	C4H+C2H2=C6H2+H	9.60E+13	0	0	
2886	C4H+O=C2H+C2O	5.00E+13	0	0	
2887	C4H+O2=HCCO+C2O	5.00E+13	0	1500	
2888	C4H+H2=H+C4H2	4.90E+05	2.5	560	
2889	C4H2+H=n-C4H3	1.10E+42	-8.72	15300	
2890	H+C4H2=i-C4H3	6.30E+46	-10.15	13500	
2891	C4H2+OH=H2C4O+H	6.60E+12	0	-410	
2892	C4H2+OH=C4H+H2O	3.37E+07	2	14000	
2893	C4H2+CH=C5H2+H	5.00E+13	0	0	
2894	C4H2+CH2=C5H3+H	1.30E+13	0	6620	
2895	C4H2+CH2*=C5H3+H	2.00E+13	0	0	
2896	C4H2+C2H=C6H2+H	9.60E+13	0	0	
2897	C4H2+C2H=C6H3	4.50E+37	-7.68	7100	
2898	H2C4O+H=C2H2+HCCO	5.00E+13	0	3000	
2899	H2C4O+OH=CH2CO+HCCO	1.00E+07	2	2000	
2900	H2C4O+O=CH2CO+C2O	2.00E+07	1.9	200	
2901	n-C4H3=i-C4H3	4.10E+43	-9.49	53000	
2902	n-C4H3+H=i-C4H3+H	2.50E+20	-1.67	10800	
2903	n-C4H3+H=2C2H2	6.30E+25	-3.34	10014	
2904	i-C4H3+H=2C2H2	2.80E+23	-2.55	10780	
2905	n-C4H3+H=C4H4	2.00E+47	-10.26	13070	
2906	i-C4H3+H=C4H4	3.40E+43	-9.01	12120	
2907	n-C4H3+H=C4H2+H2	1.50E+13	0	0	
2908	n-C4H3+OH=C4H2+H2O	2.50E+12	0	0	
2909	i-C4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0	
2910	n-C4H3+C2H2=l-C6H4+H	2.50E+14	-0.56	10600	
2911	n-C4H3+C2H2=n-C6H5	2.70E+36	-7.62	16200	
2912	n-C4H3+C2H2=A1-	9.60E+70	-17.77	31300	

(cont. on next page)

Table B .1. (cont.)

2913	n-C4H3+C2H2=c-C6H4+H	6.90E+46	-10.01	30100	
2914	C4H4+H=n-C4H3+H2	6.65E+05	2.53	12240	
2915	C4H4+OH=n-C4H3+H2O	3.10E+06	2	3430	
2916	C4H4+OH=i-C4H3+H2O	1.55E+06	2	430	
2917	C4H4+O=C3H4-P+CO	3.00E+13	0	1808	
2918	C4H4+C2H3=l-C6H6+H	2.80E+21	-2.44	14720	
2919	C4H5-N=C4H5-I	1.50E+67	-16.89	59100	
2920	C4H5-N+H=C4H5-I+H	3.10E+26	-3.35	17423	
2921	C4H6=C4H5-I+H	5.70E+36	-6.27	112353	
2922	C4H6=C4H5-N+H	5.30E+44	-8.62	123608	
2923	C4H5-I+H=C4H4+H2	3.00E+13	0	0	
2924	C4H5-I+OH=C4H4+H2O	5.00E+12	0	0	
2925	C4H5-N+O2=>C2H4+CO+HCO	4.16E+10	0	2500	
2926	C4H5-I+O2=CH2CO+CH2CHO	7.86E+16	-1.8	0	
2927	C4H5-N+C2H2=n-C6H7	1.10E+14	-1.27	2900	
2928	C4H5-N+C2H2=C6H7	5.00E+24	-5.46	4600	
2929	C4H5-N+C2H2=l-C6H6+H	5.80E+08	1.02	10900	
2930	C4H6+C2H3=C6H8+H	2.80E+21	-2.44	14720	
2931	C4H612+H=C4H6+H	2.00E+13	0	4000	
2932	C4H612+H=C3H4-A+CH3	2.00E+13	0	2000	
2933	C4H612+O=CH2CO+C2H4	1.20E+08	1.65	327	
2934	C4H612+O=C4H5-I+OH	1.80E+11	0.7	5880	
2935	C5H2+OH=>C4H2+H+CO	2.00E+13	0	0	
2936	C5H2+CH=C6H2+H	5.00E+13	0	0	
2937	C5H2+O2=H2C4O+CO	1.00E+12	0	0	
2938	C5H3+OH=C5H2+H2O	1.00E+13	0	0	
2939	C5H3+CH=C6H2+2H	5.00E+13	0	0	
2940	C5H3+CH2=l-C6H4+H	5.00E+13	0	0	
2941	C5H3+O2=H2C4O+HCO	1.00E+12	0	0	
2942	C6H+H(+M)=C6H2(+M)	1.00E+17	-1	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.75E33 -4.8E0 1.9E3/ TROE/6.464E-1 1.32E2 1.315E3 5.566E3/
2943	C6H2+H=C6H3	1.10E+30	-4.92	10800	
2944	C6H+O=C4H+C2O	5.00E+13	0	0	
2945	C6H+H2=H+C6H2	4.90E+05	2.5	560	
2946	C6H2+O=C5H2+CO	2.70E+13	0	1720	
2947	C6H2+OH=>C2H+C2H2+C2O	6.60E+12	0	-410	
2948	C6H2+OH=C6H+H2O	3.37E+07	2	14000	
2949	C6H3+H=C4H2+C2H2	2.80E+23	-2.55	10780	
2950	C6H3+H=l-C6H4	3.40E+43	-9.01	12120	
2951	C6H3+H=C6H2+H2	3.00E+13	0	0	
2952	C6H3+OH=C6H2+H2O	5.00E+12	0	0	
2953	C6H3+O2=>CO+C3H2+HCCO	5.00E+11	0	0	
2954	l-C6H4+H=n-C6H5	5.90E+39	-8.25	15600	
2955	l-C6H4+H=A1-	1.70E+78	-19.72	31400	

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Table B .1. (cont.)

2956	l-C6H4+H=c-C6H4+H	1.40E+54	-11.7	34500	
2957	l-C6H4+H=C6H3+H2	6.65E+05	2.53	9240	
2958	l-C6H4+OH=C6H3+H2O	3.10E+06	2	430	
2959	c-C6H4+H=A1-	2.40E+60	-13.66	29500	
2960	n-C6H5=A1-	5.10E+54	-13.11	35700	
2961	n-C6H5=c-C6H4+H	1.30E+59	-13.56	62000	
2962	n-C6H5+H=i-C6H5+H	2.50E+20	-1.67	10800	
2963	n-C6H5+H=C4H4+C2H2	6.30E+25	-3.34	10014	
2964	i-C6H5+H=C4H4+C2H2	2.80E+23	-2.55	10780	
2965	n-C6H5+H=l-C6H6	2.00E+47	-10.26	13070	
2966	i-C6H5+H=l-C6H6	3.40E+43	-9.01	12120	
2967	n-C6H5+H=l-C6H4+H2	1.50E+13	0	0	
2968	i-C6H5+H=l-C6H4+H2	3.00E+13	0	0	
2969	n-C6H5+OH=l-C6H4+H2O	2.50E+12	0	0	
2970	i-C6H5+OH=l-C6H4+H2O	5.00E+12	0	0	
2971	n-C6H5+O2=>C4H4+CO+HCO	4.16E+10	0	2500	
2972	i-C6H5+O2=>2CH2CO+C2H	7.86E+16	-1.8	0	
2973	l-C6H6+H=n-C6H7	1.50E+16	-1.69	1600	
2974	l-C6H6+H=C6H7	4.70E+27	-6.11	3800	
2975	l-C6H6+H=A1+H	2.00E+18	-1.73	4500	
2976	l-C6H6+H=n-C6H5+H2	6.65E+05	2.53	12240	
2977	l-C6H6+H=i-C6H5+H2	3.33E+05	2.53	9240	
2978	l-C6H6+OH=n-C6H5+H2O	6.20E+06	2	3430	
2979	l-C6H6+OH=i-C6H5+H2O	3.10E+06	2	430	
2980	n-C6H7=C6H7	1.20E+31	-7.95	8900	
2981	n-C6H7=A1+H	3.20E+26	-4.99	15500	
2982	n-C6H7+H=i-C6H7+H	2.40E+49	-10.72	15100	
2983	i-C6H7+H=C6H8	1.80E+39	-7.62	11000	
2984	n-C6H7+H=C6H8	5.60E+48	-10.54	14700	
2985	n-C6H7+H=l-C6H6+H2	1.50E+13	0	0	
2986	i-C6H7+H=l-C6H6+H2	3.00E+13	0	0	
2987	n-C6H7+OH=l-C6H6+H2O	2.50E+12	0	0	
2988	i-C6H7+OH=l-C6H6+H2O	5.00E+12	0	0	
2989	n-C6H7+O2=>C4H6+CO+HCO	4.16E+10	0	2500	
2990	i-C6H7+O2=>2CH2CO+C2H3	7.86E+16	-1.8	0	
2991	C6H8+H=n-C6H7+H2	1.33E+06	2.53	12240	
2992	C6H8+H=i-C6H7+H2	6.65E+05	2.53	9240	
2993	C6H8+OH=n-C6H7+H2O	6.20E+06	2	3430	
2994	C6H8+OH=i-C6H7+H2O	3.10E+06	2	430	
2995	A1+OH=A1-+H2O	1.60E+08	1.42	1450	
2996	A1-+H(+M)=A1(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
2997	n-C4H3+C4H2=A1C2H*	9.60E+70	-17.77	31300	
2998	A1+C2H=A1C2H+H	5.00E+13	0	0	

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Table B .1. (cont.)

2999	A1-+C2H2=n-A1C2H2	7.00E+38	-8.02	16400	
3000	A1-+C2H2=A1C2H+H	3.30E+33	-5.7	25500	
3001	A1C2H+H=n-A1C2H2	3.00E+43	-9.22	15272	
3002	A1C2H+H=i-A1C2H2	3.00E+43	-9.22	15272	
3003	A1C2H+OH=A1C2H*+H2O	1.60E+08	1.42	1450	
3004	A1C2H*+H(+M)=A1C2H(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
3005	A1+C2H3=A1C2H3+H	7.90E+11	0	6400	
3006	A1-+C2H3=A1C2H3	1.20E+27	-4.22	7235	
3007	A1-+C2H3=i-A1C2H2+H	8.50E-02	4.71	18424	
3008	A1-+C2H3=n-A1C2H2+H	9.40E+00	4.14	23234	
3009	A1C2H3=i-A1C2H2+H	5.30E+27	-3.63	109332	
3010	A1C2H3=n-A1C2H2+H	1.10E+32	-4.77	119483	
3011	A1C2H3+OH=A1C2H3*+H2O	1.60E+08	1.42	1450	
3012	A1C2H3*+H(+M)=A1C2H3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
3013	A1C2H3+H=n-A1C2H2+H2	6.65E+05	2.53	12240	
3014	A1C2H3+OH=n-A1C2H2+H2O	3.10E+06	2	3430	
3015	n-A1C2H2+H=A1C2H+H2	1.50E+13	0	0	
3016	i-A1C2H2+H=A1C2H+H2	3.00E+13	0	0	
3017	n-A1C2H2+H=i-A1C2H2+H	9.90E+04	3.37	22040	
3018	n-A1C2H2+OH=A1C2H+H2O	2.50E+12	0	0	
3019	i-A1C2H2+OH=A1C2H+H2O	5.00E+12	0	0	
3020	A1C2H*+C2H2=A1C2H)2+H	1.80E+19	-1.67	18800	
3021	A1C2H*+C2H2=naphthyne+H	5.70E+64	-14.41	57000	
3022	A1C2H)2+H=A2-1	6.90E+63	-14.57	29900	
3023	A1C2H)2+H=naphthyne+H	1.90E+73	-16.3	60900	
3024	naphthyne+H=A2-1	4.90E+52	-12.43	33000	
3025	A1C2H+C2H=A1C2H)2+H	5.00E+13	0	0	
3026	A1C2H3*+C2H2=A2+H	1.60E+16	-1.33	6600	
3027	n-A1C2H2+C2H2=A2+H	1.60E+16	-1.33	5400	
3028	A2+H=A2-2+H2	2.50E+14	0	16000	
3029	A2+OH=A2-1+H2O	1.60E+08	1.42	1450	
3030	A2+OH=A2-2+H2O	1.60E+08	1.42	1450	
3031	A2-1+H(+M)=A2(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.8E127 -3.1434E1 1.8676E4/ TROE/2.0E-1 1.228E2 4.784E2 5.4119E3/

(cont. on next page)

Table B .1. (cont.)

3032	A2-2+H(+M)=A2(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/9.5E129 -3.2132E1 1.8782E4/ TROE/8.7E-1 4.927E2 1.179E2 5.652E3/
3033	A2-1+H=A2-2+H	2.40E+24	-1.81	45281	
3034	A2+C2H=A2C2HA+H	5.00E+13	0	0	
3035	A2+C2H=A2C2HB+H	5.00E+13	0	0	
3036	A2-1+C2H2=A2C2H2	1.70E+43	-9.12	21100	
3037	A2C2HA+H=A2C2H2	5.90E+46	-10.03	19100	
3038	A2C2H2+H=A2C2HA+H2	1.50E+13	0	0	
3039	A2C2H2+OH=A2C2HA+H2O	2.50E+12	0	0	
3040	A2C2HA+OH=A2C2HA-J2+H2O	1.60E+08	1.42	1450	
3041	A2C2HB+OH=A2C2HB-J1+H2O	1.60E+08	1.42	1450	
3042	A2C2HB-J1+H(+M)=A2C2HB(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.8E127 -3.1434E1 1.8676E4/ TROE/2.0E-1 1.228E2 4.784E2 5.4119E3/
3043	A2C2HA-J2+H(+M)=A2C2HA(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/9.5E129 -3.2132E1 1.8782E4/ TROE/8.7E-1 4.927E2 1.179E2 5.652E3/
3044	A2C2HB-J1+C2H2=A2C2H)2+H	1.80E+19	-1.67	18800	
3045	A2C2H)2+H=A3-1	6.90E+63	-14.57	29900	
3046	A2C2HA-J2+C2H2=A2C2H)2+H	1.80E+19	-1.67	18800	
3047	A2C2H)2+H=A3-4	6.90E+63	-14.57	29900	
3048	A2C2HA+C2H=A2C2H)2+H	5.00E+13	0	0	
3049	A2C2HB+C2H=A2C2H)2+H	5.00E+13	0	0	
3050	A3+OH=A3-1+H2O	1.60E+08	1.42	1450	
3051	A3+OH=A3-4+H2O	1.60E+08	1.42	1450	
3052	A3-1+H(+M)=A3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/4.0E148 -3.7505E1 2.0551E4/ TROE/1.0E0 5.363E2 1.449E2 5.6328E3/
3053	A3-4+H(+M)=A3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.1E139 -3.4803E1 1.8378E4/ TROE/1.0E-3 1.714E2 1.714E2 4.9928E3/
3054	A3-1+H=A3-4+H	3.80E+40	-6.309	61782	

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Table B .1. (cont.)

3055	A3+C2H=A3C2H-4+H	5.00E+13	0	0	
3056	A3-4+C2H2=A3C2H2	8.00E+61	-14.5	34800	
3057	A3-4+C2H2=A3C2H-4+H	1.20E+26	-3.44	30200	
3058	A3C2H-4+H=A3C2H2	1.90E+64	-15.12	29300	
3059	A3C2H-4+H=A4+H	9.00E+38	-7.39	20700	
3060	A3C2H2=A4+H	1.91E+09	1.138	1629	
3061	A4+OH=A4-4+H2O	1.60E+08	1.42	1450	
3062	A4-4+H=A4	1.00E+14	0	0	
3063	A1+A1-=P2+H	1.10E+23	-2.92	15890	
3064	A1+A1-=P2-H	3.70E+32	-6.74	9870	
3065	P2-H=P2+H	3.80E+37	-7.96	27880	
3066	2A1-=P2	2.00E+19	-2.05	2900	
3067	2A1-=P2-+H	2.30E-01	4.62	28950	
3068	P2+H=P2-+H2	2.50E+14	0	16000	
3069	P2+OH=P2-+H2O	1.60E+08	1.42	1450	
3070	A1+O=C6H5O+H	2.20E+13	0	4530	
3071	C6H5O=CO+C5H5	2.50E+11	0	43900	
3072	C6H5O+H=CO+C5H6	3.00E+13	0	0	
3073	C6H5O+O=HCO+2C2H2+CO	3.00E+13	0	0	
3074	C6H5O+H(+M)=A1OH(+M)	2.50E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/1.0E94 -2.184E1 1.388E4/ TROE/4.3E-2 3.042E2 6.0E4 5.8964E3/
3075	C5H5+H(+M)=C5H6(+M)	2.60E+14	0	0	Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: H2O /6.0/ Third body: H2 /2.0/ Third body: CH4 /2.0/ LOW/4.4E80 -1.828E1 1.2994E4/ TROE/6.8E-2 4.007E2 4.136E3 5.502E3/
3076	C5H5+O=C4H5-N+CO	1.00E+14	0	0	
3077	C5H5+OH=C5H4OH+H	5.00E+12	0	0	
3078	C5H5+HO2=C5H5O+OH	3.00E+13	0	0	
3079	C5H6+H=>C5H5+H2	6.00E+07	1.876	70.5	
3080	C5H5+H2=>C5H6+H	6.27E+03	2.273	23984	
3081	C5H6+O=C5H5+OH	1.80E+13	0	3080	
3082	C5H6+OH=C5H5+H2O	3.43E+09	1.18	-447	
3083	C5H5O+H=CH2O+2C2H2	3.00E+13	0	0	
3084	C5H5O+O=CO2+C4H5-N	3.00E+13	0	0	
3085	C5H4OH=C5H4O+H	2.10E+13	0	48000	
3086	C5H4OH+H=CH2O+2C2H2	3.00E+13	0	0	
3087	C5H4OH+O=CO2+C4H5-N	3.00E+13	0	0	
3088	C5H4O=CO+2C2H2	1.00E+15	0	78000	
3089	C5H4O+O=CO2+2C2H2	3.00E+13	0	0	
3090	A1C2H+OH=>A1-+CH2CO	2.18E-04	4.5	-1000	
3091	A1C2H)2+OH=>A1C2H*+CH2CO	2.18E-04	4.5	-1000	
3092	A2C2HA+OH=>A2-1+CH2CO	2.18E-04	4.5	-1000	

(cont. on next page)

Table B .1. (cont.)

3093	A2C2HB+OH=>A2-2+CH2CO	2.18E-04	4.5	-1000	
3094	A3C2H-4+OH=>A3-4+CH2CO	2.18E-04	4.5	-1000	
3095	A1C2H+OH=>C6H5O+C2H2	1.30E+13	0	10600	
3096	A1C2H3+OH=>C6H5O+C2H4	1.30E+13	0	10600	
3097	A1C2H)2+OH=>C4H2+C6H5O	1.30E+13	0	10600	
3098	A2+OH=>A1C2H+CH2CO+H	1.30E+13	0	10600	
3099	A2C2HA+OH=>A1C2H+H2C4O+H	1.30E+13	0	10600	
3100	A2C2HB+OH=>A1C2H+H2C4O+H	1.30E+13	0	10600	
3101	A3+OH=>A2C2HB+CH2CO+H	6.50E+12	0	10600	
3102	A3+OH=>A2C2HA+CH2CO+H	6.50E+12	0	10600	
3103	A3C2H-4+OH=>A2C2HA+H2C4O+H	6.50E+12	0	10600	
3104	A3C2H-4+OH=>A2C2HB+H2C4O+H	6.50E+12	0	10600	
3105	A4+OH=>A3-4+CH2CO	1.30E+13	0	10600	
3106	A1C2H+O=>HCCO+A1-	2.04E+07	2	1900	
3107	A1C2H)2+O=>HCCO+A1C2H*	2.04E+07	2	1900	
3108	A1C2H3+O=>A1-+CH3+CO	1.92E+07	1.83	220	
3109	A2C2HA+O=>HCCO+A2-1	2.04E+07	2	1900	
3110	A2C2HB+O=>HCCO+A2-2	2.04E+07	2	1900	
3111	A1C2H+O=>C2H+C6H5O	2.20E+13	0	4530	
3112	A1C2H3+O=>C2H3+C6H5O	2.20E+13	0	4530	
3113	A1C2H)2+O=>C6H5O+C4H	2.20E+13	0	4530	
3114	A2+O=>CH2CO+A1C2H	2.20E+13	0	4530	
3115	A2C2HA+O=>A1C2H)2+CH2CO	2.20E+13	0	4530	
3116	A2C2HB+O=>A1C2H)2+CH2CO	2.20E+13	0	4530	
3117	A3+O=>A2C2HA+CH2CO	1.10E+13	0	4530	
3118	A3+O=>A2C2HB+CH2CO	1.10E+13	0	4530	
3119	A3C2H-4+O=>A2C2HA+H2C4O	1.10E+13	0	4530	
3120	A3C2H-4+O=>A2C2HB+H2C4O	1.10E+13	0	4530	
3121	A4+O=>A3-4+HCCO	2.20E+13	0	4530	
3122	A1C2H*+O2=>l-C6H4+CO+HCO	2.10E+12	0	7470	
3123	A1C2H3*+O2=>l-C6H6+CO+HCO	2.10E+12	0	7470	
3124	n-A1C2H2+O2=>A1-+CO+CH2O	1.00E+11	0	0	
3125	A2-1+O2=>A1C2H+HCO+CO	2.10E+12	0	7470	
3126	A2-2+O2=>A1C2H+HCO+CO	2.10E+12	0	7470	
3127	A2C2HA-J2+O2=>A2-1+2CO	2.10E+12	0	7470	
3128	A2C2HB-J1+O2=>A2-2+2CO	2.10E+12	0	7470	
3129	A3-4+O2=>A2C2HB+HCO+CO	2.10E+12	0	7470	
3130	A3-1+O2=>A2C2HA+HCO+CO	2.10E+12	0	7470	
3131	H2O2+OH=H2O+HO2	2.40E+00	4.042	-2162	
3132	CH3+OH=HCOH+H2	5.48E+13	0	2981	
3133	CH3+OH=CH2O+H2	2.25E+13	0	4300	
3134	CH3+H=CH2+H2	9.00E+13	0	15100	
3135	CH3+M=CH+H2+M	6.90E+14	0	82469	
3136	CH3OH(+M)=HCOH+H2(+M)	4.15E+16	-0.15	92285	Third body: H2O /16.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/4.23E44 -7.65E0 9.2911E4/ TROE/2.5E-2 1.0E-15 8.0E3 3.0E3/

(cont. on next page)

Table B .1. (cont.)

3137	CH3O+O2=CH2O+HO2	6.30E+10	0	2600	
3138	HCOH+OH=HCO+H2O	2.00E+13	0	0	
3139	HCOH+H=CH2O+H	2.00E+14	0	0	
3140	HCOH+O=CO2+2H	5.00E+13	0	0	
3141	HCOH+O=CO+OH+H	3.00E+13	0	0	
3142	HCOH+O2=CO2+H+OH	5.00E+12	0	0	
3143	HCOH+O2=CO2+H2O	3.00E+13	0	0	
3144	CH2+CO2=CH2O+CO	1.10E+11	0	1000	
3145	CH2+O=CO+H2	3.00E+13	0	0	
3146	CH2+O2=CO2+2H	3.29E+21	-3.3	2868	
3147	CH2+O2=CO2+H2	1.01E+21	-3.3	1508	
3148	CH2+O2=CO+H2O	7.28E+19	-2.54	1809	
3149	CH2+O2=HCO+OH	1.29E+20	-3.3	284	
3150	2CH2=C2H2+2H	4.00E+13	0	0	
3151	CH2(S)+C2H2=C3H3+H	1.50E+14	0	0	
3152	CH2(S)+C2H4=C3H5-A+H	1.30E+14	0	0	
3153	CH+OH=C+H2O	4.00E+07	2	3000	
3154	C2H5+H=C2H4+H2	1.25E+14	0	8000	
3155	C2H5+OH=C2H4+H2O	4.00E+13	0	0	
3156	C2H5+HO2=CH3+CH2O+OH	3.00E+13	0	0	
3157	C2H3+C2H=2C2H2	3.00E+13	0	0	
3158	C2H3+CH=CH2+C2H2	5.00E+13	0	0	
3159	C2H3+CH3=C3H5-A+H	4.73E+02	3.7	5677	
3160	C2H3+CH3=C2H2+CH4	2.00E+13	0	0	
3161	2C2H3=C4H5-I+H	7.00E+13	0	0	
3162	2C2H3=C2H4+C2H2	1.45E+13	0	0	
3163	CH2CHO+H=CH2CO+H2	4.00E+13	0	0	
3164	CH2CHO+CH3=>C2H5+CO+H	4.90E+14	-0.5	0	
3165	chocho(+M)=CH2O+CO(+M)	4.27E+12	0	50600	LOW/8.91E16 0.0E0 4.92E4/
3166	chocho=2CO+H2	4.07E+42	-8.5	69278	
3167	chocho+OH=HCO+CO+H2O	1.00E+13	0	0	
3168	chocho+O=HCO+CO+OH	7.24E+12	0	1970	
3169	chocho+H=CH2O+HCO	1.00E+12	0	0	
3170	chocho+HO2=HCO+CO+H2O2	1.70E+12	0	10700	
3171	chocho+CH3=HCO+CO+CH4	1.74E+12	0	8440	
3172	chocho+O2=HCO+CO+HO2	1.00E+14	0	37000	
3173	CH2CO+H=CH3+CO	7.00E+12	0	3011	
3174	CH2CO+OH=CH2OH+CO	3.73E+12	0	-1013	
3175	C2H+OH=C2+H2O	4.00E+07	2	8000	
3176	C2H+O2=2CO+H	9.04E+12	0	-457	
3177	HCCO+H=CH2(S)+CO	1.00E+14	0	0	
3178	HCCO+O=CH+CO2	2.95E+13	0	1113	
3179	HCCO+O2=HCO+CO+O	2.50E+08	1	0	
3180	HCCO+O2=CO2+HCO	2.40E+11	0	-854	
3181	C2+H2=C2H+H	4.00E+05	2.4	1000	
3182	C2+O2=2CO	5.00E+13	0	0	
3183	C2+OH=C2O+H	5.00E+13	0	0	

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Table B .1. (cont.)

3184	NC3H7+H=C2H5+CH3	1.00E+14	0	0	
3185	C3H6=C2H2+CH4	2.50E+12	0	70000	
3186	C3H6=C3H4-A+H2	3.00E+13	0	80000	
3187	C3H6+OH+O2=CH3CHO+CH2O+OH	3.00E+10	0	-8280	
3188	C3H6+HCO=C3H5-A+CH2O	1.08E+07	1.9	17010	
3189	CH3CHCO+OH=C2H3CO+H2O	4.00E+06	2	0	
3190	CH3CHCO+O=C2H3CO+OH	7.60E+08	1.5	8500	
3191	CH3CHCO+H=C2H3CO+H2	2.00E+05	2.5	2500	
3192	CH3CHCO+O=CH3+HCO+CO	3.00E+07	2	0	
3193	C2H3CHO+O=CH2CO+HCO+H	5.01E+07	1.76	76	
3194	C2H3CHO+H=C2H4+HCO	2.00E+13	0	3500	
3195	C2H3CO+O=C2H3+CO2	1.00E+14	0	0	
3196	C3H5-A+HO2=C2H3CHO+H+OH	1.00E+13	0	0	
3197	C3H5-A+OH=C3H4-A+H2O	1.00E+13	0	0	
3198	C3H5-A+H=C3H4-A+H2	5.00E+13	0	0	
3199	C3H5-A+O=C2H3CHO+H	1.81E+14	0	0	
3200	C3H5-A+CH3=C3H4-A+CH4	3.02E+12	-0.32	-131	
3201	C3H5-A+C2H2=C5H6+H	2.95E+32	-5.83	25733	
3202	C3H5-A+C2H3=C5H6+2H	1.59E+65	-14	61265	
3203	C3H5-T+O2=CH3CHO+HCO	1.09E+23	-3.29	3892	
3204	C3H5-T+O2=CH3CHCO+H+O	1.60E+15	-0.78	3135	
3205	C3H5-T+O=CH3CHCO+H	1.00E+14	0	0	
3206	C3H5-T+OH=C3H4-P+H2O	1.00E+13	0	0	
3207	C3H5-T+H=C3H5-A+H	1.00E+14	0	0	
3208	C3H5-S+H=C3H5-A+H	1.00E+14	0	0	
3209	C3H5-S+O2=CH3CO+CH2O	1.09E+22	-3.29	3892	
3210	C3H5-S+O=CH2CO+CH3	1.00E+14	0	0	
3211	C3H5-S+H=C3H4-P+H2	4.00E+13	0	0	
3212	C3H5-S+OH=C3H4-P+H2O	2.00E+13	0	0	
3213	C3H4-A+CH3=C3H3+CH4	1.50E+00	3.5	5600	
3214	C3H4-P+O=C2H4+CO	1.50E+13	0	2102	
3215	C3H4-A+H(+M)=C3H5-S(+M)	8.49E+12	0	2000	LOW/1.11E34 -5.0E0 4.448E3/
3216	C3H3+C2H3=C5H5+H	9.63E+40	-7.8	28820	
3217	C3H3+H(+M)=C3H4-A(+M)	1.66E+15	-0.37	0	Third body: O2 /2.0/ Third body: H2O /5.0/ Third body: C2H2 /2.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/3.36E45 -8.52E0 6.293E3/
3218	C3H3+H(+M)=C3H4-P(+M)	1.66E+15	-0.37	0	Third body: O2 /2.0/ Third body: H2O /5.0/ Third body: C2H2 /2.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/8.78E45 -8.9E0 7.974E3/
3219	2C3H3=A1	1.30E+34	-6.5	8200	
3220	C3H3+C3H5-A=FULVENE+2H	5.56E+20	-2.535	1692	
3221	2C3H3=A1-+H	2.00E+12	0	0	
3222	CJ*CC*O+O2=HCO+chocho	3.00E+12	0	0	
3223	CJ*CC*O=C2H2+HCO	1.00E+14	0	33000	

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Table B .1. (cont.)

3224	CJ*CC*O+H=C2H3CO+H	1.00E+14	0	0	
3225	CJ*CC*O+OH=HCCCHO+H2O	1.00E+13	0	0	
3226	CJ*CC*O+H=HCCCHO+H2	2.00E+13	0	0	
3227	HCCCHO+H=C2H2+HCO	1.00E+14	0	3000	
3228	HCCCHO+OH=HCCCO+H2O	1.00E+13	0	0	
3229	HCCCHO+H=HCCCO+H2	4.00E+13	0	4200	
3230	HCCCO+O2=HCO+2CO	1.40E+09	1	0	
3231	HCCCO+H=C2H2+CO	1.00E+14	0	0	
3232	C4H8-1+O=NC3H7+HCO	1.80E+05	2.5	-1029	
3233	C4H8-1+O=C2H3CHO+CH3+H	9.67E+04	2.5	-1029	
3234	C4H8-2+O=IC3H7+HCO	2.79E+06	2.12	-1775	
3235	C4H8-2+O=CH3CO+C2H5	1.53E+07	1.87	-1476	
3236	C4H8-2+O=CH3+CH3CHCO+H	8.22E+06	1.87	-1476	
3237	C4H6+OH=C4H5-N+H2O	2.00E+07	2	5000	
3238	C4H6+OH=C4H5-I+H2O	2.00E+07	2	2000	
3239	C4H6+O=HCO+C3H5-A	6.02E+08	1.45	-858	
3240	C4H6+O=CH2CHO+C2H3	1.00E+12	0	0	
3241	C4H6+H=C4H5-N+H2	3.00E+07	2	13000	
3242	C4H6+H=C4H5-I+H2	3.00E+07	2	6000	
3243	C4H6-1+OH=CH3CHCCH+H2O	1.00E+07	2	2000	
3244	C4H6-1+H=C2H5+C2H2	1.00E+14	0	3000	
3245	C4H612+OH=C4H5-I+H2O	2.00E+07	2	1000	
3246	C4H612+OH=C4H5-2+H2O	1.00E+07	2	2000	
3247	C4H612+OH=CH3CHCCH+H2O	2.00E+07	2	2500	
3248	C4H612+H=C4H5-I+H2	5.00E+07	2	5000	
3249	C4H612+H=C4H5-2+H2	1.50E+07	2	6000	
3250	C4H612+H=CH3CHCCH+H2	3.00E+07	2	6500	
3251	CH3CHCCH+H=CH3+C3H3	1.00E+14	0	0	
3252	CH3CHCCH+O2=CH3CHCO+HCO	4.16E+10	0	2510	
3253	CH3CHCCH+OH=C4H4+H2O	3.00E+13	0	0	
3254	C4H5-I+H=CH3+C3H3	1.00E+14	0	0	
3255	C4H5-I+H=C4H5-2+H	3.00E+13	0	0	
3256	C4H5-I+C2H2=A1+H	3.00E+11	0	14900	
3257	C4H5-2+H=CH3+C3H3	1.00E+14	0	0	
3258	C4H5-2+O2=CH3CO+CH2CO	4.16E+10	0	2510	
3259	C4H5-2+H=tC4H4+H2	1.00E+14	0	8000	
3260	C4H5-2+OH=tC4H4+H2O	1.00E+13	0	0	
3261	C4H5-N+OH=C4H4+H2O	2.00E+07	2	1000	
3262	C4H5-N+H=C4H4+H2	3.00E+07	2	1000	
3263	C4H5-N+C2H2=A1+H	1.60E+16	-1.33	5400	
3264	CH3CHCCH(+M)=C4H4+H(+M)	1.00E+13	0	49000	LOW/2.0E14 0.0E0 4.1E4/
3265	C4H5-2(+M)=tC4H4+H(+M)	1.00E+13	0	56000	LOW/2.0E14 0.0E0 4.8E4/
3266	C4H5-I(+M)=C4H4+H(+M)	1.00E+14	0	50000	LOW/2.0E15 0.0E0 4.2E4/
3267	C4H5-N(+M)=C4H4+H(+M)	1.00E+14	0	37000	LOW/1.0E14 0.0E0 3.0E4/
3268	C4H5-N+O2=CJ*CC*O+CH2O	1.00E+12	0	0	
3269	C4H5-N+O2=C4H4+HO2	1.00E+07	2	10000	
3270	C4H5-2+C3H3=C6H5CH2+H	3.00E+12	0	0	
3271	CH3CHCCH+C3H3=C6H5CH2+H	3.00E+12	0	0	

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Table B .1. (cont.)

3272	2C4H5-2=CH3C6H4CH2+H	3.00E+12	0	0	
3273	2CH3CHCCH=CH3C6H4CH2+H	3.00E+12	0	0	
3274	tC4H4+OH=i-C4H3+H2O	2.00E+07	2	2000	
3275	tC4H4+H=i-C4H3+H2	3.00E+07	2	6000	
3276	C4H4+H=i-C4H3+H2	3.00E+07	2	5000	
3277	n-C4H3+O2=HCCCHO+HCO	3.00E+12	0	0	
3278	i-C4H3+OH=C4H2+H2O	3.00E+13	0	0	
3279	i-C4H3+O=CH2CO+C2H	2.00E+13	0	0	
3280	i-C4H3+O=H2C4O+H	2.00E+13	0	0	
3281	i-C4H3+H=C4H2+H2	5.00E+13	0	0	
3282	i-C4H3+CH2=C3H4-A+C2H	2.00E+13	0	0	
3283	n-C4H3(+M)=C4H2+H(+M)	1.00E+14	0	36000	LOW/1.0E14 0.0E0 3.0E4/
3284	C4H2+CH2(S)=C5H3+H	3.00E+13	0	0	
3285	C4H2+O=C3H2+CO	1.20E+12	0	0	
3286	C*CCC*C+OH=C*CCJC*C+H2O	7.00E+06	2	0	
3287	C*CCC*C+H=C*CCJC*C+H2	7.00E+06	2	5000	
3288	C*CCC*C+H=C3H5-A+C2H4	3.35E+08	1.5	2000	
3289	C5H7=C5H6+H	3.16E+15	0	36000	
3290	C5H7=C*CCJC*C	3.16E+15	0	39500	
3291	C*CCJC*C+O=C2H3CHO+C2H3	2.00E+14	0	0	
3292	C*CCJC*C+H=C*CCC*C	1.00E+14	0	0	
3293	C5H6+O2=C5H5+HO2	5.00E+13	0	35400	
3294	C5H6+HO2=C5H5+H2O2	1.99E+12	0	11660	
3295	C5H6+CH3=C5H5+CH4	3.11E+11	0	5500	
3296	C5H6+C2H3=C5H5+C2H4	6.00E+12	0	0	
3297	C5H6+C4H5-N=C5H5+C4H6	6.00E+12	0	0	
3298	C5H6+C6H5O=C5H5+A1OH	3.16E+11	0	8000	
3299	C5H5+O=C5H4O+H	1.00E+14	0	0	
3300	2C5H5=>A2+2H	1.00E+12	0	6000	
3301	C5H5O=C4H5-N+CO	2.51E+11	0	43900	
3302	A1+O2=A1-+HO2	6.30E+13	0	60000	
3303	A1+H=A1-+H2	4.98E+13	0.175	10430.21	
3304	A1-+C2H4=A1C2H3+H	7.23E+01	3.5	8345	
3305	A1-+OH=C6H5O+H	5.00E+13	0	0	
3306	A1-+O=C5H5+CO	1.00E+14	0	0	
3307	A1-+O2=C6H5O+O	2.60E+13	0	6120	
3308	A1-+O2=OC6H4O+H	3.00E+13	0	8981	
3309	OC6H4O=C5H4O+CO	1.00E+15	0	78000	
3310	C6H5O+H=A1OH	1.00E+14	0	0	
3311	C6H5O+H=C24C6H6O	1.00E+14	0	0	
3312	A1OH+OH=C6H5O+H2O	2.95E+06	2	-1310	
3313	A1OH+CH3=C6H5O+CH4	1.81E+11	0	7716	
3314	A1OH+H=C6H5O+H2	1.58E+13	0	6100	
3315	A1OH+O=C6H5O+OH	2.81E+13	0	7352	
3316	A1OH+C2H3=C2H4+C6H5O	6.00E+12	0	0	
3317	A1OH+A1-=A1+C6H5O	4.91E+12	0	4400	
3318	C24C6H6O+H=C5H7+CO	2.51E+13	0	4700	
3319	C6H5CH3=A1-+CH3	1.40E+16	0	99800	

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Table B .1. (cont.)

3320	C6H5CH3+O2=C6H5CH2+HO2	2.00E+12	0	39080	
3321	C6H5CH3+OH=C6H5CH2+H2O	1.26E+13	0	2583	
3322	C6H5CH3+O=C6H5CH2+OH	5.00E+08	1.5	8000	
3323	C6H5CH3+H=C6H5CH2+H2	3.98E+02	3.44	3120	
3324	C6H5CH3+H=A1+CH3	3.50E+13	0	3690	
3325	C6H5CH3+O=OC6H4CH3+H	1.63E+13	0	3418	
3326	C6H5CH3+CH3=CH4+C6H5CH2	3.16E+11	0	9500	
3327	C6H5CH3+A1-=A1+C6H5CH2	2.10E+12	0	4400	
3328	C6H5CH2+H=C6H5CH3	1.80E+14	0	0	
3329	C6H5CH2+A1OH=C6H5O+C6H5CH3	1.05E+11	0	9500	
3330	C6H5CH2+HOC6H4CH3=OC6H4CH3+C6H5CH3	1.05E+11	0	9500	
3331	C6H5CH2+O=A1CHO+H	2.50E+14	0	0	
3332	C6H5CH2+O=A1-+CH2O	8.00E+13	0	0	
3333	C6H5CH2+HO2=A1CHO+H+OH	2.50E+14	0	0	
3334	C6H5CH2+HO2=A1-+CH2O+OH	8.00E+13	0	0	
3335	C6H5CH2+CH3=A1C2H5	1.19E+13	0	221	
3336	C6H5CH2+C3H3=C10H10	1.00E+10	0	0	
3337	C6H5CH2+A1CHO=C6H5CH3+C6H5CO	2.77E+03	2.81	5773	
3338	C6H5CH2+OH=A1CH2OH	6.00E+13	0	0	
3339	A1CH2OH+OH=A1CHO+H2O+H	8.43E+12	0	2583	
3340	A1CH2OH+H=A1CHO+H2+H	8.00E+13	0	8235	
3341	A1CH2OH+H=A1+CH2OH	1.20E+13	0	5148	
3342	A1CH2OH+C6H5CH2=A1CHO+C6H5CH3+H	2.11E+11	0	9500	
3343	A1CH2OH+A1-=A1CHO+A1+H	1.40E+12	0	4400	
3344	A1CHO+O2=C6H5CO+HO2	1.02E+13	0	38950	
3345	A1CHO+OH=C6H5CO+H2O	1.71E+09	1.18	-447	
3346	A1CHO+H=C6H5CO+H2	5.00E+13	0	4928	
3347	A1CHO+H=A1-+CH2O	2.00E+13	0	2000	
3348	A1CHO+H=A1+HCO	1.20E+13	0	5148	
3349	A1CHO+O=C6H5CO+OH	9.04E+12	0	3080	
3350	A1CHO+CH3=CH4+C6H5CO	2.77E+03	2.81	5773	
3351	A1CHO+A1-=A1+C6H5CO	7.01E+11	0	4400	
3352	C6H5CO=A1-+CO	3.98E+14	0	29400	
3353	OC6H4CH3+H=HOC6H4CH3	2.50E+14	0	0	
3354	OC6H4CH3=A1+H+CO	2.51E+11	0	43900	
3355	HOC6H4CH3+OH=OC6H4CH3+H2O	6.00E+12	0	0	
3356	HOC6H4CH3+H=OC6H4CH3+H2	1.15E+14	0	12400	
3357	HOC6H4CH3+H=C6H5CH3+OH	2.21E+13	0	7910	
3358	HOC6H4CH3+H=A1OH+CH3	1.20E+13	0	5148	
3359	A1C2H5+OH=A1C2H3+H2O+H	8.43E+12	0	2583	
3360	A1C2H5+H=A1C2H3+H2+H	8.00E+13	0	8235	
3361	A1C2H3+H=A1C2H3*+H2	3.03E+02	3.3	5690	
3362	A1C2H3+OH=i-A1C2H2+H2O	1.00E+07	2	2000	
3363	A1C2H3+H=i-A1C2H2+H2	2.00E+07	2	6000	
3364	A1C2H+O=C6H5CCO+H	4.80E+09	1	0	
3365	C6H5CCO+O2=C6H5CO+CO2	1.00E+12	0	0	
3366	A1C2H+H=A1C2H*+H2	3.03E+02	3.3	5690	
3367	A1C2H+CH3=A1C2H*+CH4	1.67E+12	0	15057	

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Table B .1. (cont.)

3368	A1C2H*+C2H2=A2-1	1.07E+04	2.324	-657.3	
3369	A1C2H3*+CH3=C9H8+2H	2.00E+13	0	0	
3370	CH3C6H4CH3+OH=CH3C6H4CH2+H2O	2.95E+13	0	2623	
3371	CH3C6H4CH3+O=CH3C6H4CH2+OH	5.00E+08	1.5	8000	
3372	CH3C6H4CH3+H=CH3C6H4CH2+H2	3.98E+02	3.44	3120	
3373	CH3C6H4CH2+C2H2=C10H10+H	3.20E+11	0	7000	
3374	CH3C6H4CH2+C2H2=ch3indene+H	3.20E+11	0	7000	
3375	CH3C6H4CH2+H=CH3C6H4CH3	7.46E+13	0	78	
3376	CH3C6H4CH2+CH3=CH3C6H4C2H5	6.00E+12	0	221	
3377	C9H8+OH=C9H7+H2O	3.43E+09	1.18	-447	
3378	C9H8+O=C9H7+OH	1.81E+13	0	3080	
3379	C9H8+H=C9H7+H2	2.19E+08	1.77	3000	
3380	C9H7+O=n-A1C2H2+CO	1.00E+14	0	0	
3381	C9H7+HO2=n-A1C2H2+CO+OH	1.00E+13	0	0	
3382	C9H7+C5H5=A3+2H	1.00E+13	0	8000	
3383	CH3C6H4C2H5+OH=CH3C6H4C2H3+H2O+H	8.43E+12	0	2583	
3384	CH3C6H4C2H5+H=CH3C6H4C2H3+H2+H	8.00E+13	0	8235	
3385	CH3C6H4C2H3+OH=C9H8+H+H2O	1.26E+13	0	2583	
3386	CH3C6H4C2H3+H=C9H8+H+H2	3.98E+02	3.44	3120	
3387	ch3indene+OH=ch3indenyl+H2O	3.43E+09	1.18	-447	
3388	ch3indene+O=ch3indenyl+OH	1.81E+13	0	3080	
3389	ch3indene+H=ch3indenyl+H2	2.19E+08	1.77	3000	
3390	ch3indene+H=C9H8+CH3	1.20E+13	0	5200	
3391	ch3indenyl+H=ch3indene	2.00E+14	0	0	
3392	ch3indenyl+C5H5=A3CH3-4+2H	1.00E+13	0	8000	
3393	C10H10+OH=C10H9+H2O	5.00E+06	2	0	
3394	C10H10+O=C10H9+OH	7.00E+11	0.7	6000	
3395	C10H10+H=C10H9+H2	2.00E+05	2.5	2500	
3396	C10H9+H=C10H10	1.00E+14	0	0	
3397	A2+H=C10H9	5.00E+14	0	5000	
3398	A2+OH=A2OH+H	9.00E+12	0	10592	
3399	A2+O=A2O+H	1.40E+13	0	1792	
3400	A2+H=A2-1+H2	4.55E+02	3.3	5690	
3401	A2-1+O2=A2O+O	1.00E+13	0	0	
3402	A2-1+OH=A2O+H	5.00E+13	0	0	
3403	A2-1+CH3=A2CH2-1+H	2.00E+13	0	0	
3404	A2-1+C2H2=A2R5+H	1.00E+20	-2.08	12000	
3405	A2-1+C2H2=A2C2HA+H	1.17E-07	5.248	-9482	
3406	A2-1+A1-=FLTN+2H	5.00E+12	0	0	
3407	A2-1+A1=FLTN+H+H2	4.00E+11	0	4000	
3408	A2O+H=A2OH	1.00E+14	0	0	
3409	A2OH+OH=A2O+H2O	2.95E+06	2	-1312	
3410	A2OH+H=A2O+H2	1.58E+13	0	6100	
3411	A2O=C9H7+CO	7.40E+11	0	43850	
3412	A2CH3-1+OH=A2CH2-1+H2O	1.27E+13	0	2583	
3413	A2CH3-1+O=A2CH2-1+OH	5.00E+08	1.5	8000	
3414	A2CH3-1+H=A2CH2-1+H2	3.98E+02	3.44	3120	
3415	A2CH3-1+H=A2+CH3	1.20E+13	0	5148	

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Table B .1. (cont.)

3416	A2CH2-1+H=A2CH3-1	1.00E+14	0	0	
3417	A2CH3-2+OH=A2CH2-2+H2O	1.27E+13	0	2583	
3418	A2CH3-2+O=A2CH2-2+OH	5.00E+08	1.5	8000	
3419	A2CH3-2+H=A2CH2-2+H2	3.98E+02	3.44	3120	
3420	A2CH3-2+H=A2+CH3	1.20E+13	0	5148	
3421	A2CH2-2+H=A2CH3-2	1.00E+14	0	0	
3422	A2CH2-1+O=A2-1+CH2O	1.00E+14	0	0	
3423	A2CH2-1+HO2=>A2-1+CH2O+OH	1.00E+13	0	0	
3424	A2CH2-1+C2H2=bz(a)ndene+H	3.20E+11	0	7000	
3425	A2CH2-1+CH3=A2C2H5	1.19E+13	0	221	
3426	A2C2H5+OH=A2C2H3+H2O+H	8.44E+12	0	2583	
3427	A2C2H5+H=A2C2H3+H2+H	8.00E+13	0	8235	
3428	A2C2H3+OH=A2CCH2+H2O	1.00E+07	2	2000	
3429	A2C2H3+H=A2CCH2+H2	2.00E+07	2	6000	
3430	A2CCH2+OH=A2C2HA+H2O	2.00E+13	0	0	
3431	A2CCH2+H=A2C2HA+H2	5.00E+13	0	0	
3432	A2C2HA+H=A2C2HA-J2+H2	3.03E+02	3.3	5690	
3433	A2C2HA+H=A2R5+H	8.46E+21	-2.614	7062.6	
3434	A2C2HA-J2+C2H2=A3-1	1.07E+04	2.324	-657.3	
3435	FLUORENE+OH=FLUORYL+H2O	3.43E+09	1.18	-447	
3436	FLUORENE+O=FLUORYL+OH	1.81E+13	0	3080	
3437	FLUORENE+H=FLUORYL+H2	2.19E+08	1.77	3000	
3438	FLUORYL+H=FLUORENE	2.00E+14	0	0	
3439	bz(a)ndnyl+H=bz(a)ndene	2.00E+14	0	0	
3440	bz(a)ndene+OH=bz(a)ndnyl+H2O	3.43E+09	1.18	-447	
3441	bz(a)ndene+O=bz(a)ndnyl+OH	1.81E+13	0	3080	
3442	bz(a)ndene+H=bz(a)ndnyl+H2	2.19E+08	1.77	3000	
3443	bz(a)ndnyl+C5H5=CHRYSEN+2H	1.00E+13	0	8000	
3444	A3+OH=A3-9+H2O	5.43E+07	1.42	1454	
3445	A3+OH=A3OH-1+H	9.00E+12	0	10592	
3446	A3+OH=A3OH-9+H	9.00E+12	0	10592	
3447	A3+H=A3-1+H2	4.04E+02	3.3	5690	
3448	A3+H=A3-9+H2	1.01E+02	3.3	5690	
3449	A3L=A3	8.00E+12	0	65000	
3450	A3-9+H=A3	8.00E+13	0	0	
3451	A3-1+O2=A3O-1+O	1.00E+13	0	0	
3452	A3-9+O2=A3O-9+O	1.00E+13	0	0	
3453	A3OH-1+OH=A3O-1+H2O	2.95E+06	2	-1310	
3454	A3OH-1+H=A3O-1+H2	1.59E+13	0	6100	
3455	A3O-1+H=A3OH-1	1.00E+14	0	0	
3456	A3OH-9+OH=A3O-9+H2O	2.95E+06	2	-1310	
3457	A3OH-9+H=A3O-9+H2	1.59E+13	0	6100	
3458	A3O-9+H=A3OH-9	1.00E+14	0	0	
3459	A3O-1=bz(a)ndnyl+CO	7.40E+11	0	43850	
3460	A3O-9=FLUORYL+CO	7.40E+11	0	43850	
3461	A3-1+C2H2=A4+H	3.49E+10	0.557	5658	
3462	A3-4+CH3=hc4-p(def)pthn+2H	2.00E+13	0	0	
3463	A3CH3-4+OH=hc4-p(def)pthn+H2O+H	1.27E+13	0	2583	

(cont. on next page)

Table B .1. (cont.)

3464	A3CH3-4+H=hc4-p(def)pthn+H2+H	3.98E+02	3.44	3120	
3465	A3CH3-4+H=A3+CH3	1.20E+13	0	5148	
3466	hc4-p(def)pthn+OH=hc4-p(def)pthyl+H2O	3.43E+09	1.18	-447	
3467	hc4-p(def)pthn+O=hc4-p(def)pthyl+OH	1.81E+13	0	3080	
3468	hc4-p(def)pthn+H=hc4-p(def)pthyl+H2	2.19E+08	1.77	3000	
3469	hc4-p(def)pthyl+H=hc4-p(def)pthn	2.00E+14	0	0	
3470	CHRYSEN+H=BZGFLTN+H2+H	3.03E+02	3.3	5690	
3471	CHRYSEN+OH=BZGFLTN+H2O+H	1.63E+08	1.42	1454	
3472	C5H5+CH3=>ch3cy24pd	1.50E+15	-1.527	-13500	
3473	ch3cy24pd=>C5H5+CH3	6.59E+59	-13.606	82000	
3474	ch3cy24pd+H=C5H6+CH3	1.00E+13	0	1300	
3475	A1+H=ch3cy24pd1	2.39E+27	-3.92	29200	
3476	C6H7=ch3cy24pd1	5.00E+12	0	38100	
3477	ch3cy24pd1+H=ch3cy24pd	1.00E+14	0	0	
3478	ch3cy24pd1+H=C5H5+CH3	1.00E+14	0	0	
3479	C6H7=ch3dcy24pd	5.50E+10	0	23500	
3480	A1+H=C6H7	4.87E+56	-12.73	26800	
3481	ch3dcy24pd+H2=ch3cy24pd+H	4.00E+12	0	15000	
3482	FULVENE=A1	9.84E+37	-7.4	76979	
3483	FULVENE+H=A1+H	3.00E+12	0.5	2000	
3484	FULVENE+H=FULVENYL+H2	3.03E+02	3.3	5690	
3485	FULVENE+OH=FULVENYL+H2O	1.63E+08	1.42	1454	
3486	FULVENYL+H=A1-+H	1.00E+14	0	0	
3487	FULVENYL+O2=C5H4O+HCO	1.00E+12	0	0	
3488	H2+O2=2OH	1.70E+13	0	47780	
3489	O+OH+M=HO2+M	1.00E+17	0	0	
3490	H2O2+O=O2+H2O	9.55E+06	2	3970	
3491	HCO+O2=CO2+OH	3.31E+12	-0.4	0	
3492	HCO+CH3O=CH3OH+CO	9.04E+13	0	0	
3493	CH+O=C+OH	1.52E+13	0	4732	
3494	CH+O2=CO+OH	3.30E+13	0	0	
3495	CH+H2O=CH2OH	5.71E+12	0	-755	
3496	CH2(S)+H2O=CH2+H2O	3.00E+13	0	0	
3497	CH2(S)+H=CH2+H	2.00E+14	0	0	
3498	CH2(S)+H2O2=CH3O+OH	3.01E+13	0	0	
3499	CH2(S)+HCO=CO+CH3	1.81E+13	0	0	
3500	CH2(S)+CH2O=HCO+CH3	1.20E+12	0	0	
3501	CH2(S)+O=CH+OH	3.00E+14	0	11923	
3502	CH2(S)+M=CH2+M	1.00E+13	0	0	Third body: H2O /0.0/ Third body: C2H2 /0.0/ Third body: H /0.0/
3503	CH2+CH3O=CH3+CH2O	1.81E+13	0	0	
3504	CH3+O=HCO+H2	1.26E+13	0	0	
3505	CH3+O=CH3O	7.96E+15	-2.12	623	
3506	CH3+CH2OH=CH4+CH2O	2.41E+12	0	0	
3507	2CH3=C2H4+H2	1.00E+16	0	32030	
3508	CH2OH+HCO=CH3OH+CO	1.20E+14	0	0	
3509	CH3O+CO=CH3+CO2	1.57E+13	0	11797	
3510	CH3OH+M=CH2+H2O+M	7.00E+15	0	66444	

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Table B .1. (cont.)

3511	CH3OH+CH2=CH2OH+CH3	1.58E+12	0	5736	
3512	C2H+M=C2+H+M	4.68E+16	0	124000	
3513	C2H+OH=CH2+CO	1.81E+13	0	0	
3514	CH+CH2=C2H+2H	5.49E+22	-2.41	11520	
3515	HCCO+H=CH2+CO	1.00E+14	0	0	
3516	HCCO+H=HCCOH	1.81E+39	-8.039	8350	
3517	HO2+C2H=HCCO+OH	1.81E+13	0	0	
3518	C2H+O2=HCCO+O	5.00E+13	0	1500	
3519	CH2CO+O=2HCO	2.00E+13	0	2293	
3520	CH2CO+OH=CH2O+HCO	2.80E+13	0	0	
3521	CH2CO+OH=CH3O+CO	2.80E+13	0	0	
3522	C2H2+O2=C2H+HO2	1.20E+13	0	74475	
3523	CH3OH+C2H=CH3O+C2H2	1.21E+12	0	0	
3524	CH3OH+C2H=CH2OH+C2H2	6.03E+12	0	0	
3525	HO2+C2H2=CH2CO+OH	6.03E+09	0	7949	
3526	HCO+C2H=C2H2+CO	6.03E+13	0	0	
3527	CH3O+C2H=CH2O+C2H2	2.41E+13	0	0	
3528	C2H+CH2OH=C2H2+CH2O	3.61E+13	0	0	
3529	2C2H=C2H2+C2	1.81E+12	0	0	
3530	C2H+CH2=CH+C2H2	1.81E+13	0	0	
3531	C2H3+O=C2H2+OH	3.00E+13	0	0	
3532	C2H3+O=CO+CH3	3.00E+13	0	0	
3533	CH+CH2=C2H3	3.09E+14	-1.98	620	
3534	2CH2=C2H3+H	2.00E+13	0	0	
3535	CH2OH+C2H2=C2H3+CH2O	7.30E+11	0	9004	
3536	C2H3+O=HCO+CH2	3.00E+13	0	0	
3537	C2H3+CH2=CH3+C2H2	1.81E+13	0	0	
3538	2CH2=C2H4	1.11E+20	-3.43	2070	
3539	CH3O+C2H3=CH2O+C2H4	2.41E+13	0	0	
3540	CH2CO+CH2=C2H4+CO	1.60E+14	0	0	
3541	C2H3+CH2O=C2H4+HCO	5.43E+03	2.81	5862	
3542	C2H3+CH2OH=C2H4+CH2O	3.01E+13	0	0	
3543	C2H4+OH=CH3+CH2O	1.05E+12	0	-916	
3544	C2H5+O=C2H4+OH	5.00E+13	0	0	
3545	HO2+C2H5=C2H4+H2O2	3.01E+11	0	0	
3546	CH3+CH2=C2H5	1.11E+19	-3.2	1780	
3547	C2H+C2H5=C2H2+C2H4	1.81E+12	0	0	
3548	CH2+C2H5=CH3+C2H4	1.81E+13	0	0	
3549	HCO+C2H5=C2H6+CO	1.21E+14	0	0	
3550	C2H4+C2H5=C2H3+C2H6	6.32E+02	3.13	18010	
3551	CH2+C2H6=CH3+C2H5	1.20E+14	0	0	
3552	C2H6+HCO=C2H5+CH2O	4.70E+04	2.7	18233	
3553	2C2H5=C2H6+C2H4	1.39E+12	0	0	
3554	C2H3+C2H5=C2H6+C2H2	4.82E+11	0	0	
3555	C2H2+C2H5=C2H6+C2H	2.71E+11	0	23446	
3556	CH+CH2O=CH2CHO	9.64E+13	0	-517	
3557	C3H6+O=CH2CHO+CH3	1.08E+06	2.15	-795	
3558	C4H8-1+O=CH2CHO+C2H5	5.14E+06	1.95	-596	

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Table B .1. (cont.)

3559	CH2CHO=CH3CO	1.00E+13	0	47100	
3560	CH3CO+O=CH3+CO2	9.64E+12	0	0	
3561	CH3CO+OH=CH2CO+H2O	1.21E+13	0	0	
3562	CH3CO+H=CH3+HCO	3.30E+13	0	0	
3563	IC3H7+HO2=CH3CHO+CH3+OH	2.41E+13	0	0	
3564	C2H4+HO2=CH3CHO+OH	6.03E+09	0	7949	
3565	C2H3+OH=CH3CHO	3.01E+13	0	0	
3566	CH3CHO+CH3=CH3COCH3+H	1.66E+10	0	12398	
3567	C3H2+O=C2H+HCO	6.80E+13	0	0	
3568	C3H2+OH=CHCHCHO	3.01E+13	0	0	
3569	C3H3=C3H2+H	5.20E+12	0	78447	
3570	C3H3+O=C3H2+OH	3.20E+12	0	0	
3571	C2H+CH2OH=C3H3+OH	1.21E+13	0	0	
3572	C2H2+HCCO=C3H3+CO	1.10E+11	0	3000	
3573	C3H3+O=C2H+CH2O	7.17E+13	0	0	
3574	C3H3+O=HCCCHO+H	6.03E+13	0	0	
3575	C3H2+O=HCCCHO	6.62E+12	0	3060	
3576	CHCHCHO+H=HCCCHO+H2	1.21E+13	0	0	
3577	CHCHCHO+OH=HCCCHO+H2O	2.00E+13	0	0	
3578	C2H+CH3CO=CH3+HCCCO	1.81E+13	0	0	
3579	HCCCHO=C2H2+CO	8.51E+14	0	70940	
3580	HCCCHO+O=HCCCO+OH	5.68E+12	0	1542	
3581	C2H+CO=HCCCO	1.51E+11	0	4810	
3582	C3H3+OH=C2H3CHO	3.01E+13	0	0	
3583	C3H4-A+O=CH2CHCO+H	6.62E+12	0	3060	
3584	C2H3+CH3CO=CH3+CH2CHCO	1.81E+13	0	0	
3585	C2H3CHO+O=CH2CHCO+OH	5.68E+12	0	1542	
3586	C2H3CHO+OH=CH2CHCO+H2O	1.60E+13	0	0	
3587	C2H3CHO+C2H5=CH2CHCO+C2H6	1.20E+13	0	12647	
3588	C2H3CHO+IC3H7=CH2CHCO+C3H8	1.02E+10	0	6840	
3589	C2H3+CO=CH2CHCO	1.51E+11	0	4810	
3590	C2H3CHO+H=CHCHCHO+H2	5.07E+07	1.93	12951	
3591	C2H3CHO+OH=CHCHCHO+H2O	2.02E+13	0	5955	
3592	C2H3CHO+CH3=CHCHCHO+CH4	4.16E+12	0	11128	
3593	CHCHCHO+H=C2H3CHO	5.36E+14	0	982	
3594	CHCHCHO=C2H2+HCO	2.95E+12	0	11110	
3595	NC3H7+O=C2H5CHO+H	9.64E+13	0	0	
3596	NC3H7+O2=C2H5CHO+OH	1.10E+08	0	0	
3597	C3H5-A+OH=C2H5CHO	3.01E+13	0	0	
3598	C3H4-A=C3H3+H	2.30E+12	0	69684	
3599	C3H4-P=C3H3+H	1.34E+12	0	69942	
3600	CH+C2H4=C3H4-A+H	7.17E+16	-0.84	1260	
3601	CH2+C2H2=C3H4CY	5.34E+34	-7.11	5830	
3602	CH2+C2H2=C3H4-A	1.04E+37	-7.42	6750	
3603	CH2+C2H2=C3H4-P	3.71E+37	-7.5	6850	
3604	C3H4CY=C3H4-A	1.51E+14	0	50400	
3605	C3H4CY=C3H4-P	7.08E+13	0	43700	
3606	C3H4-A+OH=HCO+C2H4	1.00E+12	0	0	

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Table B .1. (cont.)

3607	C2H+CH3=C3H4-P	8.27E+46	-10	46330	
3608	C2H3+CH2=C3H4-A+H	3.00E+13	0	0	
3609	C3H4-P+C2H=C2H2+C3H3	1.00E+13	0	0	
3610	C3H4-A+O=HCO+C2H3	9.00E+12	0	1870	
3611	C3H4-P+O=CH2O+C2H2	7.50E+12	0	2102	
3612	CH+C2H4=C3H5-A	2.42E+37	-8.04	4840	
3613	C3H5-A+CH2=C4H6+H	3.01E+13	0	0	
3614	C2H+C3H5-A=C2H2+C3H4-A	1.50E-01	0	0	
3615	C2H+C3H5-A=C2H3+C3H3	2.00E+01	0	0	
3616	C2H3+CH2OH=C3H5-A+OH	1.21E+13	0	0	
3617	C2H4+CH2=C3H5-A+H	3.19E+12	0	5285.4	
3618	C3H6+CH2OH=C3H5-A+CH3OH	6.03E+01	2.95	11989	
3619	C3H6+CH3O=C3H5-A+CH3OH	9.00E+01	2.95	11987	
3620	C3H6+C2H=C3H4-P+C2H3	1.21E+13	0	0	
3621	C3H6+CH2=C3H5-A+CH3	7.23E+11	0	6192	
3622	C3H6+C2H3=C3H5-A+C2H4	2.21E+00	3.5	4682	
3623	C3H5-A+HCO=C3H6+CO	6.03E+13	0	0	
3624	C3H5-A+CH2OH=C3H6+CH2O	1.81E+13	0	0	
3625	C3H5-A+CH3O=C3H6+CH2O	3.01E+13	0	0	
3626	C3H5-A+C2H3=C3H6+C2H2	4.82E+12	0	0	
3627	CH2+C2H5=C3H6+H	9.03E+12	0	0	
3628	CH2+C2H4=C3H6	9.03E+13	0	0	
3629	NC3H7+H=C3H6+H2	1.81E+12	0	0	
3630	NC3H7+OH=C3H6+H2O	2.41E+13	0	0	
3631	NC3H7+CH2=C3H6+CH3	1.81E+12	0	0	
3632	NC3H7+CH3=C3H6+CH4	1.14E+13	-0.32	0	
3633	NC3H7+CH2OH=C3H6+CH3OH	4.82E+11	0	0	
3634	NC3H7+C2H=C3H6+C2H2	6.03E+12	0	0	
3635	NC3H7+C2H3=C3H6+C2H4	1.21E+12	0	0	
3636	NC3H7+C2H5=C3H6+C2H6	1.45E+12	0	0	
3637	NC3H7+C3H5-A=2C3H6	1.45E+12	0	-131	
3638	IC3H7+H=C3H6+H2	3.61E+12	0	0	
3639	IC3H7+CH3=C3H6+CH4	9.41E+10	0.68	0	
3640	IC3H7+C2H=C3H6+C2H2	3.61E+12	0	0	
3641	IC3H7+CH2OH=C3H6+CH3OH	2.89E+12	0	0	
3642	IC3H7+C2H3=C3H6+C2H4	1.52E+14	-0.7	0	
3643	IC3H7+C2H5=C3H6+C2H6	2.30E+13	-0.35	0	
3644	IC3H7+C3H5-A=2C3H6	2.29E+13	-0.35	-131	
3645	IC3H7=CH3+C2H4	1.00E+12	0	34580	
3646	NC3H7+CH2=C2H4+C2H5	1.81E+13	0	0	
3647	IC3H7+C2H2=C4H6+CH3	2.77E+10	0	6504	
3648	NC3H7+C2H=C3H3+C2H5	1.21E+13	0	0	
3649	NC3H7+C2H3=C2H2+C3H8	1.21E+12	0	0	
3650	NC3H7+HCO=C3H8+CO	6.03E+13	0	0	
3651	NC3H7+CH2OH=C3H8+CH2O	9.64E+11	0	0	
3652	NC3H7+CH3O=C3H8+CH2O	2.41E+13	0	0	
3653	NC3H7+CH3OH=C3H8+CH2OH	3.37E+01	3.17	9161	
3654	NC3H7+CH2O=C3H8+HCO	3.01E+03	2.9	5862	

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Table B .1. (cont.)

3655	NC3H7+C2H5=C3H8+C2H4	1.15E+12	0	0	
3656	2NC3H7=C3H8+C3H6	1.69E+12	0	0	
3657	NC3H7+C3H5-A=C3H4-A+C3H8	7.23E+11	0	-131	
3658	IC3H7+C2H5=C2H4+C3H8	1.84E+13	-0.35	0	
3659	IC3H7+CH3OH=C3H8+CH2OH	3.19E+01	3.7	10532	
3660	IC3H7+CH2O=C3H8+HCO	1.08E+11	0	6955	
3661	IC3H7+HCO=C3H8+CO	1.21E+14	0	0	
3662	IC3H7+CH2OH=C3H8+CH2O	2.35E+12	0	0	
3663	IC3H7+CH3O=C3H8+CH2O	1.21E+13	0	0	
3664	IC3H7+C2H3=C3H8+C2H2	1.52E+14	-0.7	0	
3665	IC3H7+NC3H7=C3H8+C3H6	5.13E+13	-0.35	0	
3666	2IC3H7=C3H8+C3H6	2.11E+14	-0.7	0	
3667	IC3H7+C3H5-A=C3H8+C3H4-A	4.58E+12	-0.35	-131	
3668	2C3H2=C4H2+C2H2	2.00E+13	0	85000	
3669	C4H2+C2H=C4H+C2H2	2.00E+13	0	0	
3670	C4H4+C2H=C4H2+C2H3	1.00E+13	0	0	
3671	i-C4H3+H2=C2H2+C2H3	5.01E+10	0	20000	
3672	C3H3+CH=n-C4H3+H	7.00E+13	0	0	
3673	2C2H2=C4H4	1.66E+45	-9.46	58460	
3674	2C2H3=C4H4+2H	7.83E+12	0	0	
3675	C4H4+C2H=i-C4H3+C2H2	4.00E+13	0	0	
3676	C4H4+C2H=n-C4H3+C2H2	4.00E+13	0	0	
3677	C2H3+C2H=C4H4	9.10E+45	-9.118	21130	
3678	C4H4+C2H3=C2H4+n-C4H3	5.00E+11	0	16300	
3679	C4H4+C2H3=C2H4+i-C4H3	5.00E+11	0	16300	
3680	C4H5-I+O2=C4H4+HO2	1.20E+11	0	0	
3681	C2H3+C2H4=I-C4H7	1.32E+27	-5.58	4000	
3682	I-C4H7=C4H6+H	3.16E+13	0	34800	
3683	I-C4H7+H=C4H6+H2	1.81E+12	0	0	
3684	I-C4H7+OH=C4H6+H2O	2.41E+13	0	0	
3685	C3H6+C2H3=C4H6+CH3	7.23E+11	0	5010	
3686	C4H6+C3H3=C4H5-N+C3H4-A	1.00E+13	0	22500	
3687	C3H3+CH3=C4H6-1	5.42E+13	0	0	
3688	C3H6+C2H=C4H6-1+CH	1.21E+13	0	0	
3689	C4H6-1=C4H612	2.50E+13	0	65000	
3690	C4H6-1+O=C3H6+CO	2.00E+13	0	1659	
3691	C3H3+CH3=C4H612	3.61E+13	0	0	
3692	C4H612=C4H6	2.50E+13	0	63000	
3693	C4H612+H=C3H4-P+CH3	6.00E+12	0	2100	
3694	I-C4H7+H=C4H8-1	1.00E+14	0	0	
3695	C5H4CY+H=C5H3CY+H2	1.00E+06	2.5	5000	
3696	C5H4CY+OH=C5H3CY+H2O	1.00E+06	2	0	
3697	C5H4CY+O=C5H3CY+OH	1.00E+06	2.5	3000	
3698	C5H3CY+H=C5H4CY	1.00E+14	0	0	
3699	C5H3CY+O2=C2H2+HCCO+CO	1.00E+12	0	0	
3700	C5H3+H=C5H2+H2	6.03E+13	0	15103	
3701	C5H5+H=C5H4CY+H2	3.23E+07	2.095	15842	
3702	C5H5+OH=C5H4CY+H2O	2.11E+13	0	4571	

(cont. on next page)

Table B .1. (cont.)

3703	C5H5+O=C5H4CY+OH	2.00E+13	0	14694	
3704	C5H5+CH3=C5H4CY+CH4	2.00E+12	0	15060	
3705	C5H4H+H=C5H4CY+H2	2.80E+13	0	2259	
3706	C5H4H+OH=C5H4CY+H2O	3.08E+06	2	0	
3707	C5H4H+O=C5H4CY+OH	4.77E+04	2.71	1106	
3708	C5H4CY=C5H4L	1.00E+13	0	6000	
3709	C5H5L+H=C5H4L+H2	1.81E+12	0	0	
3710	C5H5L+OH=C5H4L+H2O	2.41E+13	0	0	
3711	C5H5L+CH3=C5H4L+CH4	1.95E+13	-0.5	0	
3712	C5H5=C3H3+C2H2	1.98E+68	-15	124887	
3713	C5H5=C5H4H	5.92E+78	-19.5	96689	
3714	C5H4H=C3H3+C2H2	7.48E+65	-15	92201	
3715	C5H5=C5H5L	2.52E+80	-18.9	129171	
3716	C5H5+O=C5H5O	7.06E+04	1.03	-6960	
3717	C5H5O=C5H4O+H	2.90E+32	-6.5	21220	
3718	C5H4OH+O2=C5H4O+HO2	3.00E+13	0	5000	
3719	C5H4O+H=C4H5-N+CO	2.10E+61	-13.27	40810	
3720	C5H4O+O=C4H4+CO2	1.00E+13	0	2000	
3721	C5H6+H=C5H4H+H2	2.80E+13	0	35139	
3722	C5H6+OH=C5H4H+H2O	3.08E+06	2	32880	
3723	C5H6+O=C5H4H+OH	4.77E+04	2.71	33986	
3724	C5H6+CH3=C5H4H+CH4	1.80E-01	4	32880	
3725	C5H6+A1-=C5H5+A1	1.00E-01	4	0	
3726	C5H6+A2-1=C5H5+A2	1.00E-01	4	0	
3727	C5H6+A2-2=C5H5+A2	1.00E-01	4	0	
3728	C5H6+C4H5-I=C5H5+C4H6	6.00E+12	0	0	
3729	C5H6+C3H5-A=C5H5+C3H6	2.00E-01	4	0	
3730	C3H5-A+C5H5=C5H6+C3H4-A	1.00E+12	0	0	
3731	C6H2+C2H=C6H+C2H2	2.00E+13	0	0	
3732	C6H2+C2H=C4H+C4H2	1.00E+13	0	0	
3733	2C3H2=C6H2+H2	2.00E+13	0	85000	
3734	l-C6H4+C2H=C6H3+C2H2	2.00E+13	0	0	
3735	i-C4H3+C2H3=A1-+H	6.00E+12	0	0	
3736	A1-+HO2=C6H5O+OH	5.00E+13	0	1000	
3737	A1-+CH2O=A1+HCO	1.75E+10	0	0	
3738	A1-+H=c-C6H4+H2	9.17E-22	10.28	6175	
3739	C4H4+C2H3=A1+H	1.90E+12	0	2510	
3740	A1+C3H3=>A1-+C3H4-A	2.27E+01	3.517	24065	
3741	A1-+C3H4-A=>A1+C3H3	2.58E+00	3.73	899.32	
3742	C4H5-N+C2H3=A1+H2	1.84E-13	7.07	-3610	
3743	C4H4+C2H2=A1	4.47E+11	0	30010	
3744	A1+O=A1-+OH	2.00E+13	0	14704	
3745	A1-+CH4=>A1+CH3	5.15E+03	2.896	15307.6	
3746	A1+CH3=>A1-+CH4	2.24E+02	3.202	6620.8	
3747	A1+OH=A1OH+H	1.56E+24	-3.19	16900	
3748	CH3+C5H5=C6H7+H	2.44E+41	-7.989	39259	
3749	C6H7+H=A1+H2	1.00E+13	0	0	
3750	C6H7+A1-=2A1	1.00E+12	0	0	

(cont. on next page)

Table B .1. (cont.)

3751	C6H7+H=C6H813	6.00E+13	0	0	
3752	C6H7+H=C6H814	6.00E+13	0	0	
3753	2C6H7=C6H813+A1	1.94E+15	-1	0	
3754	2C6H7=C6H814+A1	1.67E+15	-1	0	
3755	C6H813+O2=C6H7+HO2	8.13E+11	0	24840	
3756	C6H814+H=C6H7+H2	2.80E+13	0	2259	
3757	C6H813=A1+H2	4.70E+13	0	61600	
3758	C6H814=A1+H2	1.05E+12	0	42690	
3759	C2H3+C4H5-N=C6H813	8.53E+13	-1.11	820	
3760	C4H6+C2H2=C6H814	2.30E+12	0	35000	
3761	C6H5O+O=C5H5+CO2	1.00E+13	0	0	
3762	A1OH=C5H6+CO	1.00E+12	0	60802	
3763	A1OH+HO2=C6H5O+H2O2	3.00E+13	0	15000	
3764	A1OH+C4H5-N=C4H6+C6H5O	6.00E+12	0	0	
3765	A1OH+C4H5-I=C4H6+C6H5O	6.00E+12	0	0	
3766	A1OH+OH=H2O+C6H4OH	1.41E+13	0	4571	
3767	A1OH+H=H2+C6H4OH	1.67E+14	0	16000	
3768	C5H5+CO=C6H4OH	4.48E+10	-0.805	51190	
3769	C6H5O+O=OC6H4O+H	8.50E+13	0	0	
3770	C6H5O+O=PC6H4O2+H	8.50E+13	0	0	
3771	PC6H4O2=C5H4O+CO	3.70E+11	0	59000	
3772	PC6H4O2=C5H4CY+CO2	3.50E+12	0	67000	
3773	PC6H4O2+H=C5H5O+CO	2.50E+13	0	4700	
3774	PC6H4O2+H=C6H3O2+H2	2.00E+12	0	8100	
3775	PC6H4O2+O=C6H3O3+H	1.50E+13	0	4530	
3776	PC6H4O2+O=C6H3O2+OH	1.40E+13	0	14700	
3777	PC6H4O2+OH=C6H3O2+H2O	1.00E+06	2	4000	
3778	C6H3O2+H=PC6H4O2	1.00E+14	0	0	
3779	C6H3O2+H=2C2H2+2CO	1.00E+14	0	0	
3780	C6H3O2+O=C2H2+HCCO+2CO	1.00E+14	0	0	
3781	C6H3O3=C2H2+HCCO+2CO	1.00E+12	0	50000	
3782	C6H3O3+H=C2H2+CH2CO+2CO	1.00E+14	0	0	
3783	A1-+CH3=C6H5CH2+H	3.61E+17	-0.76	20250	
3784	C4H4+C3H3=C6H5CH2	7.25E+18	-2.77	-13860	
3785	C6H5CH3+C2H3=C6H5CH2+C2H4	3.98E+12	0	8000	
3786	C4H5-N+C3H4-A=C6H5CH3+H	2.00E+11	0	3700	
3787	C4H5-N+C3H4-P=C6H5CH3+H	3.16E+11	0	3700	
3788	C6H5O+CH3=HOC6H4CH3	1.00E+12	0	0	
3789	A1CHO=C6H5CO+H	3.98E+15	0	83660	
3790	C6H5O+CH3=C6H5OCH3	1.21E+13	0	0	
3791	A1-+CH3O=C6H5OCH3	1.21E+13	0	0	
3792	A1-+C6H5O=C6H5OC6H5	1.21E+13	0	0	
3793	A1-+C2H=A1C2H	2.54E+17	-1.489	1541	
3794	A1-+C4H4=A1C2H+C2H3	3.20E+11	0	1350	
3795	C4H5-N+C4H2=A1C2H+H	3.16E+11	0	1800	
3796	A1C2H+O=C6H5CH+CO	3.60E+12	0	633	
3797	C6H5CH+H=C6H5CH2	1.00E+13	0	0	
3798	C6H5CH2+H=C6H5CH+H2	6.03E+13	0	15103	

(cont. on next page)

Table B .1. (cont.)

3799	C6H5CH+O=A1+CO	1.00E+13	0	0	
3800	C6H5CH+OH=A1+HCO	1.00E+13	0	0	
3801	A1C2H+OH=A1+HCCO	2.44E+03	3.02	11076	
3802	A1-+C4H4=A1C2H3+C2H	3.20E+11	0	1900	
3803	A1-+C4H6=A1C2H3+C2H3	3.20E+11	0	1900	
3804	2C4H4=A1C2H3	1.50E+14	0	38000	
3805	C4H5-N+C4H4=A1C2H3+H	3.16E+11	0	600	
3806	A1C2H3=A1+C2H2	1.58E+11	0	58440	
3807	A1-+C2H2=C8H7*2	1.10E+41	-8.61	18152	
3808	C8H7*2+H=A1C2H3	1.11E+16	-0.817	690	
3809	A1C2H3+H=C8H7*2+H2	3.23E+07	2.095	15842	
3810	A1C2H3+OH=C8H7*2+H2O	2.11E+13	0	4571	
3811	C8H7*2+O2=C6H5O+CH2CO	1.88E+12	0	7469	
3812	A1C2H3+O=A1-+CH2CHO	3.50E+13	0	2832	
3813	A1C2H3+O=n-A1C2H2+OH	7.55E+06	1.91	3736	
3814	A1C2H5+H=A1+C2H5	1.20E+13	0	5100	
3815	A1C2H5+H=A1C2H4+H2	3.97E+02	3.44	3120	
3816	A1C2H5+OH=A1C2H4+H2O	5.17E+09	1	870	
3817	A1C2H5+O2=A1C2H4+HO2	1.81E+12	0	39740	
3818	A1C2H5=A1C2H4+H	2.51E+15	0	81262	
3819	A1C2H4=A1C2H3+H	3.16E+13	0	50669	
3820	A1-+C3H3=A1C3H2+H	3.00E+12	0	0	
3821	A1C3H2+C3H3=P2-+H	3.00E+12	0	0	
3822	P2-+H=P2	2.50E+20	-1.79	2880	
3823	C8H7*2+C2H2=A2+H	4.67E+06	1.787	3262	
3824	A1-+n-C4H3=A2	6.62E+35	-6.485	15420	
3825	C6H5CH2+C3H3=A2+2H	3.00E+12	0	0	
3826	A1-+n-C4H3=A2-2+H	2.43E+31	-4.541	36700	
3827	A2+CH3=A2-1+CH4	2.00E+12	0	15060	
3828	A2+CH3=A2-2+CH4	2.00E+12	0	15060	
3829	A2-1+H=naphthyne1+H2	9.17E-22	10.28	6175	
3830	A2-2+H=naphthyne2+H2	9.17E-22	10.28	6175	
3831	naphthyne1+c-C6H4=A21C6H4	3.20E+23	-3.22	5070	
3832	naphthyne2+c-C6H4=A22C6H4	3.20E+23	-3.22	5070	
3833	A2-1+O2=A2O-1+O	3.40E+30	-5.1	12950	
3834	A2-1+OH=A2O-1+H	5.00E+13	0	0	
3835	A2-2+O2=A2O-2+O	3.40E+30	-5.1	12950	
3836	A2-2+OH=A2O-2+H	5.00E+13	0	0	
3837	A2O-1+H=A2OH-1	3.47E+29	-4.303	10230	
3838	A2OH-1+H=A2O-1+H2	1.15E+14	0	12400	
3839	A2+OH=A2OH-1+H	1.56E+24	-3.19	16900	
3840	A2OH-1+OH=A2O-1+H2O	1.39E+08	1.43	-962	
3841	A2O-2+H=A2OH-2	3.47E+29	-4.303	10230	
3842	A2OH-2+H=A2O-2+H2	1.15E+14	0	12400	
3843	A2+OH=A2OH-2+H	1.56E+24	-3.19	16900	
3844	A2OH-2+OH=A2O-2+H2O	1.39E+08	1.43	-962	
3845	A2O-1=C9H7+CO	2.51E+11	0	43900	
3846	A2O-2=C9H7+CO	2.51E+11	0	43900	

(cont. on next page)

Table B .1. (cont.)

3847	A2-2+CH3=A2CH2-2+H	6.30E+14	0.26	27320	
3848	A2-1+CH3=A2CH3-1	1.85E+32	-5.7	8890	
3849	A2-2+CH3=A2CH3-2	1.85E+32	-5.7	8890	
3850	A2-2+C2H2=A2C2HB+H	3.89E+17	-0.87	19780	
3851	A2VINP+H=A2C2HB+H2	9.57E+14	-0.25	720	
3852	A2-2+C2H4=A2C2H3-2+H	2.51E+12	0	6200	
3853	A2+C2H3=A2C2H3-2+H	7.94E+11	0	6399	
3854	A2-2+C2H2=A2VINP	1.16E+35	-7.04	11720	
3855	A2VINP=A2C2HB+H	2.74E+22	-4.061	37040	
3856	A2VINP+H=A2C2H3-2	1.54E+13	-0.99	-6880	
3857	2c-C6H4=BIPHEN	4.60E+12	0	0	
3858	BIPHENH=BIPHEN+H	1.30E+16	0	33203	
3859	BIPHENH+H=BIPHEN+H2	6.02E+12	0	0	
3860	BIPHENH=A2R5+H	1.00E+13	0	20000	
3861	A2R5+H=A2R5J1+H2	3.23E+07	2.095	19800	
3862	A2R5+H=A2R5J3+H2	3.23E+07	2.095	15842	
3863	A2R5+H=A2R5J4+H2	3.23E+07	2.095	15842	
3864	A2R5+H=A2R5J5+H2	3.23E+07	2.095	15842	
3865	A2R5+OH=A2R5J1+H2O	2.10E+13	0	8600	
3866	A2R5+OH=A2R5J3+H2O	2.10E+13	0	4600	
3867	A2R5+OH=A2R5J4+H2O	2.10E+13	0	4600	
3868	A2R5+OH=A2R5J5+H2O	2.10E+13	0	4600	
3869	A2R5J1+H=A2R5	1.26E+20	-1.81	2900	
3870	A2R5J1+H=A2R5T+H2	1.92E-14	8.65	18600	
3871	A2R5J1+OH=A2R5T+H2O	1.00E+13	0	0	
3872	A2R5J1+O=A2R5T+OH	1.00E+13	0	0	
3873	A2R5J3+H=A2R5	7.00E+19	-1.73	2790	
3874	A2R5J4+H=A2R5	7.00E+19	-1.73	2790	
3875	A2R5J5+H=A2R5	7.00E+19	-1.73	2790	
3876	A2-1+C2H4=A2R5H2+H	2.51E+12	0	6200	
3877	A2-1+C2H2=HA2R5	4.60E+41	-9	15525	
3878	HA2R5+H=A2R5+H2	1.81E+12	0	0	
3879	HA2R5+OH=A2R5+H2O	2.41E+13	0	0	
3880	HA2R5+H=A2R5H2	1.00E+14	0	0	
3881	A2R5H2+H=HA2R5+H2	5.40E+02	3.5	5210	
3882	A2R5H2+OH=HA2R5+H2O	8.70E+09	1.05	1810	
3883	A2R5H2=A2R5+H2	4.70E+13	0	61600	
3884	A2R5J1+C2H2=A2R5E1+H	1.51E+17	-0.72	20230	
3885	A2R5J3+C2H2=A2R5E3+H	1.51E+17	-0.72	20230	
3886	A2R5J4+C2H2=A2R5E4+H	1.51E+17	-0.72	20230	
3887	A2R5J5+C2H2=A2R5E5+H	4.43E-06	5.71	11070	
3888	A2R5J5+C2H2=A2R5R5+H	4.11E+15	-0.443	14420	
3889	P2-+C2H2=A3+H	1.87E+07	1.787	3262	
3890	A2C2HB+H=A2C2HB-J1+H2	3.23E+07	2.095	15842	
3891	A2C2HB-J1+C2H2=A3-1	4.67E+06	1.787	3262	
3892	A2C2HA-J2+C2H2=A3-4	4.67E+06	1.787	3262	
3893	A1C2H+A1-=A3+H	9.55E+11	0	4308	
3894	A1C2H*+A1=A3+H	9.55E+11	0	4308	

(cont. on next page)

Table B .1. (cont.)

3895	A3+H=A3-2+H2	3.23E+07	2.095	15842	
3896	A3+H=A3-4+H2	3.23E+07	2.095	15842	
3897	A3+OH=A3-2+H2O	2.11E+13	0	4571	
3898	A3-2+H=A3	2.02E+15	-0.3	330	
3899	A2C2HB+H=A2C2HB-J3+H2	3.23E+07	2.095	15842	
3900	A2C2HB+OH=A2C2HB-J3+H2O	2.11E+13	0	4571	
3901	A2C2HB-J3+C2H2=A3L-1	4.67E+06	1.787	3262	
3902	A2-2+C4H2=A3L-2	4.67E+06	1.787	3262	
3903	A3L+H=A3L-1+H2	3.23E+07	2.095	15842	
3904	A3L+OH=A3L-1+H2O	2.11E+13	0	4571	
3905	A3L-1+H=A3L	2.02E+15	-0.3	330	
3906	A3L+H=A3L-2+H2	3.23E+07	2.095	15842	
3907	A3L+OH=A3L-2+H2O	2.11E+13	0	4571	
3908	A3L-2+H=A3L	2.02E+15	-0.3	330	
3909	A3L+H=A3L-9+H2	3.23E+07	2.095	15842	
3910	A3L+OH=A3L-9+H2O	2.11E+13	0	4571	
3911	A3L-9+H=A3L	2.02E+15	-0.3	330	
3912	A3-1+C2H2=A3R5+H	1.83E+13	0.295	14940	
3913	naphthyne1+c-C6H4=A3R5	2.64E+32	-4.88	42450	
3914	naphthyne2+c-C6H4=A3R5	2.64E+32	-4.88	42450	
3915	A2R5E4+H=A2R5E4J5+H2	3.23E+07	2.095	15842	
3916	A2R5E4+OH=A2R5E4J5+H2O	2.10E+13	0	4600	
3917	A2R5E4J5+C2H2=A3R5J7	1.87E+07	1.787	3262	
3918	A3R5J7+H=A3R5	5.00E+13	0	0	
3919	A2R5E5+H=A2R5E5J4+H2	3.23E+07	2.095	15842	
3920	A2R5E5+OH=A2R5E5J4+H2O	2.10E+13	0	4600	
3921	A2R5E5J4+C2H2=A3R5J10	1.87E+07	1.787	3262	
3922	A3R5J10+H=A3R5	5.00E+13	0	0	
3923	A3L-1+C2H2=A3LR5+H	1.83E+13	0.295	14940	
3924	A3L-9+C2H2=A3LR5+H	1.87E+07	1.787	3262	
3925	naphthyne1+c-C6H4=A3LR5	3.09E+36	-6.29	42180	
3926	naphthyne2+c-C6H4=A3LR5	3.09E+36	-6.29	42180	
3927	A2R5E3+H=A2R5E3J4+H2	3.23E+07	2.095	15842	
3928	A2R5E3+OH=A2R5E3J4+H2O	2.10E+13	0	4600	
3929	A2R5E4+H=A2R5E4J3+H2	3.23E+07	2.095	15842	
3930	A2R5E4+OH=A2R5E4J3+H2O	2.10E+13	0	4600	
3931	A2R5E3J4+C2H2=A3LR5J	1.87E+07	1.787	3262	
3932	A2R5E4J3+C2H2=A3LR5J	1.87E+07	1.787	3262	
3933	A3LR5J+H=A3LR5	5.00E+13	0	0	
3934	A3-2+C2H2=A3C2H-2+H	2.08E+15	-0.13	20860	
3935	A3C2H-2+H=A3C2H-2J3+H2	3.23E+07	2.095	15842	
3936	A3C2H-2+OH=A3C2H-2J3+H2O	2.10E+13	0	4600	
3937	A3C2H-2J3+C2H2=CHRYSENJ1	1.87E+07	1.787	3262	
3938	A3-1+C2H2=A3C2H-1+H	4.63E-07	6.03	11850	
3939	A3C2H-1+H=A3C2H-1J2+H2	3.23E+07	2.095	15842	
3940	A3C2H-1+OH=A3C2H-1J2+H2O	2.10E+13	0	4600	
3941	A3C2H-1J2+C2H2=CHRYSENJ4	1.87E+07	1.787	3262	
3942	A2-2+A1C2H=CHRYSEN+H	8.51E+11	0	3986	

(cont. on next page)

Table B .1. (cont.)

3943	A2+A1C2H*=CHRYSEN+H	8.51E+11	0	3986	
3944	A2C2HA-J2+A1=CHRYSEN+H	8.51E+11	0	3986	
3945	CHRYSEN+H=CHRYSENJ1+H2	3.23E+07	2.095	15842	
3946	CHRYSEN+H=CHRYSENJ4+H2	3.23E+07	2.095	15842	
3947	CHRYSEN+H=CHRYSENJ5+H2	3.23E+07	2.095	15842	
3948	CHRYSEN+OH=CHRYSENJ1+H2O	2.10E+13	0	4600	
3949	CHRYSEN+OH=CHRYSENJ4+H2O	2.10E+13	0	4600	
3950	CHRYSEN+OH=CHRYSENJ5+H2O	2.10E+13	0	4600	
3951	CHRYSENJ1+H=CHRYSEN	5.00E+13	0	0	
3952	CHRYSENJ4+H=CHRYSEN	5.00E+13	0	0	
3953	CHRYSENJ5+H=CHRYSEN	5.00E+13	0	0	
3954	CHRYSENJ4+C2H2=BAPYR+H	1.87E+07	1.787	3262	
3955	CHRYSENJ5+C2H2=BAPYR+H	1.87E+07	1.787	3262	
3956	A3L-1+C2H2=A3LC2H-1+H	4.63E-07	6.03	11850	
3957	A3LC2H-1+H=A3LC2H-1J2+H2	3.23E+07	2.095	15842	
3958	A3LC2H-1+OH=A3LC2H-1J2+H2O	2.10E+13	0	4600	
3959	A3LC2H-1J2+C2H2=BA3L-1	1.87E+07	1.787	3262	
3960	A3L-2+C2H2=A3LC2H-2+H	2.08E+15	-0.13	20860	
3961	A3LC2H-2+H=A3LC2H-2J1+H2	3.23E+07	2.095	15842	
3962	A3LC2H-2+OH=A3LC2H-2J1+H2O	2.10E+13	0	4600	
3963	A3LC2H-2J1+C2H2=BA3L-4	1.87E+07	1.787	3262	
3964	A2-2+A1C2H=BA3L+H	8.51E+11	0	3986	
3965	A2+A1C2H*=BA3L+H	8.51E+11	0	3986	
3966	BA3L+H=BA3L-1+H2	3.23E+07	2.095	15842	
3967	BA3L+H=BA3L-12+H2	3.23E+07	2.095	15842	
3968	BA3L+H=BA3L-4+H2	3.23E+07	2.095	15842	
3969	BA3L+OH=BA3L-1+H2O	2.10E+13	0	4600	
3970	BA3L+OH=BA3L-12+H2O	2.10E+13	0	4600	
3971	BA3L+OH=BA3L-4+H2O	2.10E+13	0	4600	
3972	BA3L-1+H=BA3L	5.00E+13	0	0	
3973	BA3L-4+H=BA3L	5.00E+13	0	0	
3974	BA3L-12+H=BA3L	5.00E+13	0	0	
3975	A3LC2H-2+H=A3LC2H-2J3+H2	3.23E+07	2.095	15842	
3976	A3LC2H-2+OH=A3LC2H-2J3+H2O	2.10E+13	0	4600	
3977	A3LC2H-2J3+C2H2=A4LJS	1.87E+07	1.787	3262	
3978	A4LJS+H=A4L	5.00E+13	0	0	
3979	A3-1+A1-=BBFLTN+2H	5.00E+12	0	0	
3980	A3-1+A1=BBFLTN+H2+H	4.00E+11	0	4000	
3981	A3-9+A1-=BBFLTN+2H	5.00E+12	0	0	
3982	A3-9+A1=BBFLTN+H2+H	4.00E+11	0	4000	
3983	A2-2+A2-1=BKFLTN+2H	5.00E+12	0	0	
3984	A2+A2-2=BKFLTN+H2+H	4.00E+11	0	4000	
3985	A2+A2-1=BKFLTN+H2+H	4.00E+11	0	4000	
3986	A4-1+A1-=INPYR+2H	5.00E+12	0	0	
3987	A4-1+A1=INPYR+H2+H	4.00E+11	0	4000	
3988	BBFLTN+H=BBFLTNJS+H2	3.23E+07	2.095	15842	
3989	BBFLTN+OH=BBFLTNJS+H2O	2.10E+13	0	4600	
3990	BBFLTNJS+C2H2=INPYR+H	1.87E+07	1.787	3262	

(cont. on next page)

Table B .1. (cont.)

3991	A3-4+CH3=A3CH2+H	5.00E+13	0	0	
3992	A3CH2+H=A3CH3-4	1.00E+14	0	0	
3993	A3CH3-4+H=A3CH2+H2	3.98E+02	3.44	3120	
3994	A3CH3-4+OH=A3CH2+H2O	1.26E+13	0	2583	
3995	A3CH2=A3CH2R+H	1.00E+13	0	12000	
3996	A2+C6H5CH2=BENZNAP+H	1.20E+12	0	15940	
3997	A2-2+C6H5CH2=BENZNAP	1.19E+13	0	220	
3998	BENZNAP+H=BENZNAPJP+H2	3.23E+07	2.095	15842	
3999	BENZNAP+OH=BENZNAPJP+H2O	2.10E+13	0	4600	
4000	BENZNAPJP=C17H12+H	1.00E+13	0	12000	
4001	A1+C6H5CH2=BENZYLB+H	1.20E+12	0	15940	
4002	A1-+C6H5CH2=BENZYLB	1.19E+13	0	220	
4003	BENZYLB+H=BENZYLBJ+H2	3.23E+07	2.095	15842	
4004	BENZYLB+OH=BENZYLBJ+H2O	2.10E+13	0	4600	
4005	BENZYLBJ=FLUORENE+H	4.00E+11	0	12000	
4006	A2-2+A1-=A2C6H5-2	1.19E+17	-1.16	1990	
4007	A2-2+A1=A2C6H5-2+H	2.22E+83	-20.79	46890	
4008	A2+A1-=A2C6H5-2+H	2.22E+83	-20.79	46890	
4009	A2+A1-=FLTN+H+H2	8.51E+11	0	3986	
4010	naphthyne1+c-C6H4=FLTN	1.34E+23	-2.76	22470	
4011	naphthyne2+c-C6H4=FLTN	1.34E+23	-2.76	22470	
4012	A2R5E1+H=A2R5E1J2+H2	3.23E+07	2.095	15842	
4013	A2R5E1+OH=A2R5E1J2+H2O	2.10E+13	0	4600	
4014	A2R5E1J2+C2H2=FLTNJ7	1.87E+07	1.787	3262	
4015	FLTN+H=FLTNJ1+H2	3.23E+07	2.095	15842	
4016	FLTN+OH=FLTNJ1+H2O	2.10E+13	0	4600	
4017	FLTN+H=FLTNJ3+H2	3.23E+07	2.095	15842	
4018	FLTN+OH=FLTNJ3+H2O	2.10E+13	0	4600	
4019	FLTNJ7+H=FLTN	5.00E+13	0	0	
4020	FLTNJ1+H=FLTN	5.00E+13	0	0	
4021	FLTNJ3+H=FLTN	5.00E+13	0	0	
4022	A21C6H4=FLTN	8.51E+12	0	62860	
4023	A22C6H4=A3LR5	8.51E+12	0	62860	
4024	A3R5=FLTN	8.51E+12	0	62860	
4025	A3LR5=A3R5	8.51E+12	0	62860	
4026	A3LR5=FLTN	8.51E+12	0	62860	
4027	FLTNJ3+C2H2=CPCFLTN+H	1.43E+13	0.353	15790	
4028	CPCFLTN+H=CPCFLTNJS+H2	3.23E+07	2.095	15842	
4029	CPCFLTN+OH=CPCFLTNJS+H2O	2.10E+13	0	4600	
4030	CPCFLTNJS+C2H2=CPBZFLTN+H	1.87E+07	1.787	3262	
4031	BZGFLTN-+C2H2=CPBZFLTN+H	1.43E+13	0.353	15790	
4032	CPBZFLTN+H=CPBZFLTNJS+H2	3.23E+07	2.095	15842	
4033	CPBZFLTN+OH=CPBZFLTNJS+H2O	2.10E+13	0	4600	
4034	CPBZFLTNJS+C2H2=COR1+H	1.87E+07	1.787	3262	
4035	A3-4+C2H2=A4+H	1.87E+07	1.787	3262	
4036	A1C2H*+A1C2H=A4+H	8.51E+11	0	3986	
4037	A4+OH=A4-1+H2O	1.60E+08	1.42	1450	
4038	A4+OH=A4-2+H2O	2.10E+13	0	4600	

(cont. on next page)

Table B .1. (cont.)

4039	A4-2+H=A4	1.00E+14	0	0	
4040	A4-4+O2=A3-4+2CO	2.10E+12	0	7470	
4041	A4-1+C2H2=A4C2H-1+H	7.92E-06	5.71	13330	
4042	A4-2+C2H2=A4C2H-2+H	1.25E+17	-0.56	22560	
4043	A4-4+C2H2=A4C2H-4+H	7.92E-06	5.71	13330	
4044	FLTNJ1+C2H2=BZGFLTN+H	1.87E+07	1.787	3262	
4045	FLTNJ7+C2H2=BZGFLTN+H	1.87E+07	1.787	3262	
4046	BZGFLTN+H=BZGFLTN-+H2	3.23E+07	2.095	15842	
4047	BZGFLTN+OH=BZGFLTN-+H2O	2.10E+13	0	4600	
4048	A4-1+C2H2=CPCDA4+H	1.43E+13	0.353	15790	
4049	A4-4+C2H2=CPCDA4+H	1.43E+13	0.353	15790	
4050	CPCDA4+H=CPCDA4-+H2	3.23E+07	2.095	15842	
4051	CPCDA4+OH=CPCDA4-+H2O	2.10E+13	0	4600	
4052	CPCDA4-+C2H2=DCPCDA4+H	1.43E+13	0.353	15790	
4053	BZGFLTN-+C2H2=COR+H	1.87E+07	1.787	3262	
4054	CPCDA4-+C2H2=COR+H	1.43E+13	0.353	15790	
4055	COR+H=COR-+H2	3.23E+07	2.095	15842	
4056	COR+OH=COR-+H2O	2.10E+13	0	4600	
4057	COR-+C2H2=COR1+H	1.43E+13	0.353	15790	
4058	COR1+H=COR1-+H2	3.23E+07	2.095	15842	
4059	COR1+OH=COR1-+H2O	2.10E+13	0	4600	
4060	COR1-+C2H2=COR2+H	1.87E+07	1.787	3262	
4061	COR2+H=COR2-+H2	3.23E+07	2.095	15842	
4062	COR2+OH=COR2-+H2O	2.10E+13	0	4600	
4063	COR2-+C2H2=COR3+H	1.87E+07	1.787	3262	
4064	COR3+H=COR3-+H2	3.23E+07	2.095	15842	
4065	COR3+OH=COR3-+H2O	2.10E+13	0	4600	
4066	COR3-+C2H2=COR4+H	1.87E+07	1.787	3262	
4067	COR4+H=COR4-+H2	3.23E+07	2.095	15842	
4068	COR4+OH=COR4-+H2O	2.10E+13	0	4600	
4069	COR4-+C2H2=HB+H	1.87E+07	1.787	3262	
4070	BA3L-1+C2H2=BAPYR+H	1.87E+07	1.787	3262	
4071	BA3L-12+C2H2=BAPYR+H	1.87E+07	1.787	3262	
4072	A4C2H-1+H=A4C2H-1J2+H2	3.23E+07	2.095	15842	
4073	A4C2H-1+OH=A4C2H-1J2+H2O	2.10E+13	0	4600	
4074	A4C2H-2+H=A4C2H-2J1+H2	3.23E+07	2.095	15842	
4075	A4C2H-2+OH=A4C2H-2J1+H2O	2.10E+13	0	4600	
4076	A4C2H-1J2+C2H2=BAPYRJS	1.87E+07	1.787	3262	
4077	A4C2H-2J1+C2H2=BAPYRJS	1.87E+07	1.787	3262	
4078	BAPYRJS+H=BAPYR	5.00E+13	0	0	
4079	A2C2HA-J2+A1C2H=BAPYR+H	8.51E+11	0	3986	
4080	A2C2HA+A1C2H*=BAPYR+H	8.51E+11	0	3986	
4081	BAPYR+OH=A4C2H-2+CH2CO+H	6.50E+12	0	10600	
4082	BAPYR+O=A4C2H-2+CH2CO	1.10E+13	0	4530	
4083	BAPYRJS+O2=A4C2H-2+HCO+CO	2.10E+12	0	7470	
4084	A4C2H-2+OH=A4-2+CH2CO	2.18E-04	4.5	-1000	
4085	A4C2H-2+O=A4-2+HCCO	2.04E+07	2	1900	
4086	A4C2H-4+H=A4C2H-4J5+H2	3.23E+07	2.095	15842	

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Table B .1. (cont.)

4087	A4C2H-4+OH=A4C2H-4J5+H2O	2.10E+13	0	4600	
4088	A4C2H-4J5+C2H2=BEPYRJS	1.87E+07	1.787	3262	
4089	BEPYRJS+H=BEPYR	5.00E+13	0	0	
4090	BEPYR+H=BEPYRJS+H2	3.23E+07	2.095	15842	
4091	BEPYR+OH=BEPYRJS+H2O	2.10E+13	0	4600	
4092	BEPYRJS+C2H2=BGHIPER+H	1.87E+07	1.787	3262	
4093	2A2-1=PERYLEN+2H	1.39E+13	0	111	
4094	A2-1+A2=PERYLEN+H2+H	8.51E+11	0	3986	
4095	PERYLEN+H=PERYLENJS+H2	3.23E+07	2.095	15842	
4096	PERYLEN+OH=PERYLENJS+H2O	2.10E+13	0	4600	
4097	PERYLENJS+C2H2=BGHIPER+H	1.87E+07	1.787	3262	
4098	BGHIPER+H=BGHIPEJS1+H2	3.23E+07	2.095	15842	
4099	BGHIPER+OH=BGHIPEJS1+H2O	2.10E+13	0	4600	
4100	BGHIPEJS1+C2H2=CPBPER+H	1.43E+13	0.353	15790	
4101	BAPYR+H=BAPYRJS+H2	3.23E+07	2.095	15842	
4102	BAPYR+OH=BAPYRJS+H2O	2.10E+13	0	4600	
4103	BAPYRJS+C2H2=ANTHAN+H	1.87E+07	1.787	3262	
4104	ANTHAN+H=ANTHANJS+H2	3.23E+07	2.095	15842	
4105	ANTHAN+OH=ANTHANJS+H2O	2.10E+13	0	4600	
4106	ANTHAN+OH=BAPYRJS+CH2CO	1.30E+13	0	10600	
4107	ANTHAN+O=BAPYRJS+HCCO	2.20E+13	0	4530	
4108	ANTHANJS+O2=BAPYRJS+2CO	2.10E+12	0	7470	
4109	C6H5CH2=FC7H6+H	4.38E+13	0.078	75900	
4110	C6H5CH2+H=FC7H6+H2	5.00E+13	0	0	
4111	FC7H6+H=>C5H5+C2H2	3.00E+14	0	0	
4112	FC7H5+H=FC7H6	2.00E+12	0	0	
4113	FC7H6+CH3=FC7H5+CH4	1.87E+04	2.724	6008	
4114	FC7H6+H=FC7H5+H2	1.90E+08	1.847	4965	
4115	FC7H5+H=C5H4CY+C2H2	1.00E+14	0	0	
4116	FC7H5(+M)=C4H2+C3H3(+M)	3.00E+12	-0.075	62300	LOW/1.0E45 8.4E0 4.75E4/
4117	FC7H5(+M)=C2H2+C5H3(+M)	2.00E+11	-0.075	62300	LOW/1.0E45 8.4E0 4.75E4/
4118	A2-1+O=A2O	1.00E+14	0	0	
4119	A2-2+O=A2O	1.00E+14	0	0	
4120	A2-2+O2=A2O+O	8.90E+03	2.4	38277.51	
4121	A2-2+OH=A2O+H	3.00E+13	0	0	
4122	A2OH+O=A2O+OH	2.81E+13	0	7351.8	
4123	A2O+O=C9H6O+CO+H	1.68E+14	0	0	
4124	A2O+O2=C9H6O+CO+OH	1.08E+12	0.1	17999.5	
4125	C9H7+C3H3=A2R5+H2	4.10E+43	-9.2	15153	
4126	C9H7+HO2=C9H6O+H2O	4.76E+32	-6.5	13401	
4127	C9H7+HO2=>C9H6O+H+OH	1.31E+29	-4.7	11649.1	
4128	C9H7+O=C9H6O+H	2.80E+13	0	0	
4129	C9H7+O2=C9H6O+OH	1.38E+11	0	25320.3	
4130	C9H7+O2=>C9H6O+H+O	3.09E+15	-0.7	48740.4	
4131	C9H8+O=>C9H6O+2H	6.65E+12	-0.1	360.9	
4132	C6H5CH2+C2H2=C9H8+H	3.16E+04	2.5	11061.2	
4133	C9H8=C9H7+H	1.73E+68	-15.2	116371.9	
4134	C9H6O+H=>A1C2H3*+CO	1.79E+07	2.1	841.3	

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Table B .1. (cont.)

4135	C9H8+HCO=C9H7+CH2O	1.08E+08	1.9	15999	
4136	C9H8+HO2=C9H7+H2O2	1.10E+04	2.6	12899.1	
4137	C9H8+O2=C9H7+HO2	4.00E+13	0	49639.1	
4138	C9H8+OH=>O-C6H4+C2H4+HCO	1.88E+36	-7.8	7060.2	
4139	FC7H6+C2H2=C9H8	1.44E+292	-78.2	245010	
4140	FC7H6+C2H2=C9H7+H	9.70E-42	16.7	37520	
4141	A1-+C3H4-A=C9H8+H	5.13E+02	3.2	2788	
4142	A1-+C3H3=C9H8	1.50E+75	-17.8	39600	
4143	A1+C3H3=C9H8+H	6.26E+09	2.61	56500	
4144	C9H8+CH3=>C9H7+CH4	2.75E+00	3.614	3380.1	
4145	C9H7+CH4=>C9H8+CH3	1.10E-02	3.883	29788	
4146	C9H8+C3H3=>C9H7+C3H4-A	5.15E-03	4.376	8021.8	
4147	C9H7+C3H4-A=>C9H8+C3H3	2.63E-03	4.563	18582	
4148	C6H5CH2=C5H5+C2H2	2.00E+14	0	70000	
4149	C5H6+H=C*CCJC*C	1.10E+14	-0.16	3100	
4150	C*CCJC*C+O2=C2H3CHO+CH2CHO	1.20E+36	-7.25	33600	
4151	C4H6-2=C4H6	3.00E+13	0	65000	
4152	C4H6-2=C4H612	3.00E+13	0	67000	
4153	C4H6-2+H=C4H612+H	2.00E+13	0	4000	
4154	C4H6-2+H=C4H5-2+H2	3.40E+05	2.5	2490	
4155	C4H6-2+H=CH3+C3H4-P	2.60E+05	2.5	1000	
4156	C4H6-2=H+C4H5-2	5.00E+15	0	87300	
4157	C4H6-2+CH3=C4H5-2+CH4	1.40E+14	0	18500	
4158	C4H5-2+C2H4=C5H6+CH3	5.00E+14	0	25000	
4159	C4H5-2+HO2=>OH+C2H2+CH3CO	8.00E+11	0	0	
4160	A4+CH3=>A4-1+CH4	7.98E-01	3.933	11771	
4161	A4-1+CH4=>A4+CH3	4.48E-02	4.248	4277	
4162	A4+C3H3=>A4-1+C3H4-A	1.91E+01	3.529	24449.2	
4163	A4-1+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
4164	A4+H=>A4-1+H2	4.90E+08	1.884	9829.5	
4165	A4-1+H2=>A4+H	4.90E+04	2.467	2926.4	
4166	A4-1+C4H4=>BAPYR+H	1.26E+04	2.61	1649.2	
4167	A4+CH3=>A4-2+CH4	7.98E-01	3.933	11771	
4168	A4-2+CH4=>A4+CH3	4.48E-02	4.248	4277	
4169	A4+C3H3=>A4-2+C3H4-A	1.91E+01	3.529	24449.2	
4170	A4-2+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
4171	A4+H=>A4-2+H2	4.90E+08	1.884	9829.5	
4172	A4-2+H2=>A4+H	4.90E+04	2.467	2926.4	
4173	A4-2+C4H4=>BAPYR+H	1.26E+04	2.61	1649.2	
4174	A4+CH3=>A4-4+CH4	7.98E-01	3.933	11771	
4175	A4-4+CH4=>A4+CH3	4.48E-02	4.248	4277	
4176	A4+C3H3=>A4-4+C3H4-A	1.91E+01	3.529	24449.2	
4177	A4-4+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
4178	A4+H=>A4-4+H2	4.90E+08	1.884	9829.5	
4179	A4-4+H2=>A4+H	4.90E+04	2.467	2926.4	
4180	A4-4+C4H4=>BEPYR+H	1.26E+04	2.61	1649.2	
4181	A2C2HA-J2+C4H4=>A4+H	3.30E+33	-5.7	12750	
4182	C6H5CH2+C9H7=>A4+2H2	2.00E+12	0	2000	

(cont. on next page)

Table B .1. (cont.)

4183	2C9H7=>A4+C2H2+H2	6.39E+29	-4.03	35205.5	
4184	A3CH2+CH2=>A4+H2+H	2.40E+14	0	0	
4185	A4-1+H=A4	1.00E+14	0	0	

Table B. 2. Skeletal kinetic mechanism reactions and their rate parameters (pre-exponent factor, temperature exponent, and activation energy)

	Reactions	A (cm, s, mol units)			
1	H+O2=O+OH	1.04E+14	0	15286	REV/2.637E4 2.651E0 4.88E3/
2	OH+H2=H+H2O	2.16E+08	1.51	3430	REV/2.29E9 1.404E0 1.832E4/
3	O2+M=2O+M	4.42E+17	-0.634	118900	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.83/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.83/ REV/6.165E15 -5.0E-1 0.0E0/
4	OH+M=O+H+M	9.78E+17	-0.743	102100	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.75/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.75/ REV/4.714E18 -1.0E0 0.0E0/
5	H+O2(+M)=HO2(+M)	1.48E+12	0.6	0	Third body: H2 /1.3/ Third body: H2O /14.0/ Third body: AR /0.67/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.67/ LOW/3.482E16 -4.11E-1 -1.115E3/ TROE/5.0E-1 1.0E-30 1.0E30 1.0E10/
6	HO2+H=H2+O2	1.66E+13	0	823	REV/3.166E12 3.48E-1 5.551E4/
7	HO2+H=2OH	7.08E+13	0	295	REV/2.028E10 7.2E-1 3.684E4/
8	HO2+O=OH+O2	3.25E+13	0	0	REV/3.217E12 3.29E-1 5.328E4/
9	HO2+OH=H2O+O2	1.97E+10	0.962	-328.4	REV/3.989E10 1.204E0 6.925E4/
10	H2O2+O2=2HO2	1.14E+16	-0.347	49730	REV/1.03E14 0.0E0 1.104E4/ DUP
11	H2O2+O2=2HO2	2.14E+13	-0.347	37280	REV/1.94E11 0.0E0 -1.409E3/ DUP
12	H2O2(+M)=2OH(+M)	2.95E+14	0	48430	Third body: H2 /2.5/ Third body: H2O /12.0/ Third body: AR /0.64/ Third body: CO /1.9/ Third body: CO2 /3.8/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.64/ LOW/1.202E17 0.0E0 4.55E4/ TROE/5.0E-1 1.0E-30 1.0E30 1.0E10/
13	H2O2+H=H2+HO2	2.15E+10	1	6000	REV/3.716E7 1.695E0 2.2E4/
14	H2O2+O=OH+HO2	9.55E+06	2	3970	REV/8.568E3 2.676E0 1.856E4/
15	CO+O(+M)=CO2(+M)	1.80E+10	0	2384	Third body: H2 /2.0/ Third body: O2 /6.0/ Third body: H2O /6.0/ Third body: AR /0.5/ Third body: CO /1.5/ Third body: CO2 /3.5/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.5/ LOW/1.35E24 -2.788E0 4.191E3/
16	CO+OH=CO2+H	6.00E+10	0.2161	-260.5	
17	CO+HO2=CO2+OH	3.01E+13	0	23000	REV/2.28E16 -4.7E-1 8.497E4/
18	HCO+M=H+CO+M	4.75E+11	0.66	14870	Third body: H2 /2.0/ Third body: H2O /12.0/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ REV/3.582E10 1.041E0 -4.573E2/
19	HCO+O2=CO+HO2	7.58E+12	0	410	REV/1.198E12 3.09E-1 3.395E4/
20	HCO+H=CO+H2	7.34E+13	0	0	REV/2.212E12 6.56E-1 8.823E4/
21	HCO+O=CO+OH	3.02E+13	0	0	REV/4.725E11 6.38E-1 8.682E4/

(cont. on next page)

Table B .2. (cont.)

22	HCO+O=CO2+H	3.00E+13	0	0	REV/1.241E18 -5.53E-1 1.122E5/
23	HCO+OH=CO+H2O	1.02E+14	0	0	pagw
24	HCO+CH3=CH4+CO	2.65E+13	0	0	REV/7.286E14 2.11E-1 8.977E4/
25	HCO+HO2=CH2O+O2	2.50E+14	-0.061	13920	REV/8.07E15 0.0E0 5.342E4/
26	HCO+HO2=>CO2+H+OH	3.00E+13	0	0	
27	CH2O+CO=2HCO	9.19E+13	0.37	73040	REV/1.8E13 0.0E0 0.0E0/
28	2HCO=>H2+2CO	3.00E+12	0	0	
29	HCO+H(+M)=CH2O(+M)	1.09E+12	0.48	-260	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.35E24 -2.57E0 1.425E3/ TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
30	CO+H2(+M)=CH2O(+M)	4.30E+07	1.5	79600	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/5.07E27 -3.42E0 8.4348E4/ TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
31	CH2O+OH=HCO+H2O	7.82E+07	1.63	-1055	REV/4.896E6 1.811E0 2.903E4/
32	CH2O+H=HCO+H2	5.74E+07	1.9	2740	REV/3.39E5 2.187E0 1.793E4/
33	CH2O+O=HCO+OH	6.26E+09	1.15	2260	REV/1.919E7 1.418E0 1.604E4/
34	CH3O(+M)=CH2O+H(+M)	6.80E+13	0	26170	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ LOW/1.867E25 -3.0E0 2.4307E4/ TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
35	CH2O+CH3O=CH3OH+HCO	6.62E+11	0	2294	REV/8.393E10 7.4E-2 1.771E4/
36	CH4+CH3O=CH3+CH3OH	6.12E+02	2.867	8248	REV/1.44E1 3.1E0 6.935E3/
37	CH3O+CH3=CH2O+CH4	1.20E+13	0	0	REV/6.749E13 2.18E-1 8.281E4/
38	CH3O+HO2=CH2O+H2O2	3.01E+11	0	0	REV/1.074E12 -3.1E-2 6.527E4/
39	CH3OH(+M)=CH3+OH(+M)	1.90E+16	0	91730	LOW/2.95E44 -7.35E0 9.546E4/ TROE/4.14E-1 2.79E2 5.459E3 1.0E10/
40	CH3OH+CH2O=2CH3O	7.98E+12	0.452	81490	REV/6.03E13 0.0E0 0.0E0/
41	H+CH3(+M)=CH4(+M)	1.20E+15	-0.4	0	Third body: H2 /2.0/ Third body: CO /2.0/ Third body: CO2 /3.0/ Third body: H2O /5.0/ LOW/6.4E23 -1.8E0 0.0E0/ SRI/4.5E-1 7.97E2 9.79E2 1.0E0 0.0E0/
42	CH4+H=CH3+H2	6.14E+05	2.5	9587	REV/6.73E2 2.946E0 8.047E3/
43	CH4+OH=CH3+H2O	5.83E+04	2.6	2190	REV/6.776E2 2.94E0 1.554E4/
44	CH4+O=CH3+OH	1.02E+09	1.5	8600	REV/5.804E5 1.927E0 5.648E3/
45	CH4+HO2=CH3+H2O2	1.13E+01	3.74	21010	REV/7.166E0 3.491E0 3.468E3/
46	CH4+CH2=2CH3	2.46E+06	2	8270	REV/1.736E6 1.868E0 1.298E4/
47	CH3+OH=CH2(S)+H2O	4.51E+17	-1.34	1417	REV/1.654E16 -8.55E-1 1.039E3/
48	CH3+OH=CH3O+H	6.94E+07	1.343	11200	REV/1.5E12 5.0E-1 -1.1E2/
49	CH3+OH=CH2+H2O	5.60E+07	1.6	5420	REV/9.224E5 2.072E0 1.406E4/
50	CH3+HO2=CH3O+OH	1.00E+12	0.269	-687.5	REV/6.19E12 1.47E-1 2.455E4/
51	CH3+HO2=CH4+O2	1.16E+05	2.23	-3022	REV/2.018E7 2.132E0 5.321E4/
52	CH3+O=CH2O+H	5.54E+13	0.05	-136	REV/3.83E15 -1.47E-1 6.841E4/
53	CH3+O2=CH3O+O	7.55E+12	0	28320	REV/4.718E14 -4.51E-1 2.88E2/

(cont. on next page)

Table B .2. (cont.)

54	CH3+O2=CH2O+OH	2.64E+00	3.283	8105	REV/5.285E-1 3.477E0 5.992E4/
55	CH3+O2(+M)=CH3O2(+M)	7.81E+09	0.9	0	LOW/6.85E24 -3.0E0 0.0E0/ TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
56	CH3O2+CH2O=CH3O2H+HCO	1.99E+12	0	11660	REV/1.323E14 -8.53E-1 9.259E3/
57	CH4+CH3O2=CH3+CH3O2H	1.81E+11	0	18480	REV/2.233E12 -6.94E-1 -6.55E2/
58	CH3O2+CH3=2CH3O	5.08E+12	0	-1411	REV/1.967E12 1.76E-1 2.807E4/
59	CH3O2+HO2=CH3O2H+O2	2.47E+11	0	-1570	REV/5.302E14 -7.92E-1 3.552E4/
60	2CH3O2=>CH2O+CH3OH+O2	3.11E+14	-1.61	-1051	
61	2CH3O2=>O2+2CH3O	1.40E+16	-1.61	1860	
62	CH3O2+H=CH3O+OH	9.60E+13	0	0	REV/1.72E9 1.019E0 4.078E4/
63	CH3O2+O=CH3O+O2	3.60E+13	0	0	REV/2.229E11 6.28E-1 5.752E4/
64	CH3O2+OH=CH3OH+O2	6.00E+13	0	0	REV/1.536E13 4.34E-1 5.916E4/
65	CH3O2H=CH3O+OH	6.31E+14	0	42300	REV/2.514E6 1.883E0 -2.875E3/
66	CH2(S)=CH2	1.00E+13	0	0	REV/4.488E12 -1.3E-2 9.02E3/
67	CH2(S)+CH4=2CH3	1.60E+13	0	-570	REV/5.067E12 -1.45E-1 1.316E4/
68	CH2(S)+O2=>CO+OH+H	7.00E+13	0	0	
69	CH2(S)+H2=CH3+H	7.00E+13	0	0	REV/2.022E16 -5.91E-1 1.527E4/
70	CH2(S)+H=CH+H2	3.00E+13	0	0	REV/6.948E13 -2.53E-1 1.248E4/
71	CH2(S)+O=>CO+2H	3.00E+13	0	0	
72	CH2(S)+OH=CH2O+H	3.00E+13	0	0	REV/1.154E18 -7.7E-1 8.523E4/
73	CH2+H(+M)=CH3(+M)	2.50E+16	-0.8	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/3.2E27 -3.14E0 1.23E3/ TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
74	CH2+O2=CH2O+O	2.40E+12	0	1500	REV/5.955E14 -3.65E-1 6.098E4/
75	CH2+O2=>CO+OH+H	5.00E+12	0	1500	
76	CH2+O=>CO+2H	5.00E+13	0	0	
77	CH2+H=CH+H2	1.00E+18	-1.56	0	REV/5.16E18 -1.8E0 3.46E3/ DUP
78	CH2+OH=CH+H2O	1.13E+07	2	3000	REV/6.183E8 1.655E0 2.135E4/
79	CH+O2=HCO+O	3.30E+13	0	0	REV/9.371E12 1.61E-1 7.121E4/
80	CH+O=CO+H	5.70E+13	0	0	REV/2.774E15 0.0E0 1.76E5/
81	CH+OH=HCO+H	3.00E+13	0	0	REV/5.069E14 0.0E0 8.811E4/
82	CH2+H=CH+H2	2.70E+11	0.67	25700	REV/1.897E11 6.7E-1 2.873E4/ DUP
83	CH+H2O=H+CH2O	1.71E+13	0	-755	REV/8.372E14 0.0E0 5.752E4/
84	2CH3(+M)=C2H6(+M)	9.21E+16	-1.17	635.8	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.135E36 -5.246E0 1.705E3/ TROE/4.05E-1 1.12E3 6.96E1 1.0E10/
85	C2H5+H(+M)=C2H6(+M)	5.21E+17	-0.99	1580	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.99E41 -7.08E0 6.685E3/ TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
86	C2H6+H=C2H5+H2	1.15E+08	1.9	7530	REV/1.062E4 2.582E0 9.76E3/
87	C2H6+O=C2H5+OH	3.55E+06	2.4	5830	REV/1.702E2 3.063E0 6.648E3/

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Table B .2. (cont.)

88	C2H6+OH=C2H5+H2O	1.48E+07	1.9	950	REV/1.45E4 2.476E0 1.807E4/
89	C2H6+O2=C2H5+HO2	6.03E+13	0	51870	REV/2.921E10 3.34E-1 -5.93E2/
90	C2H6+CH3=C2H5+CH4	1.51E-07	6	6047	REV/1.273E-8 6.236E0 9.817E3/
91	C2H6+HO2=C2H5+H2O2	3.46E+01	3.61	16920	REV/1.849E0 3.597E0 3.151E3/
92	C2H6+CH3O2=C2H5+CH3O2H	1.94E+01	3.64	17100	REV/2.017E1 3.182E0 1.734E3/
93	C2H6+CH3O=C2H5+CH3OH	2.41E+11	0	7090	REV/4.779E8 4.69E-1 9.547E3/
94	C2H6+CH=C2H5+CH2	1.10E+14	0	-260	REV/1.969E9 9.21E-1 -1.49E3/
95	CH2(S)+C2H6=CH3+C2H5	1.20E+14	0	0	REV/3.203E12 9.1E-2 1.75E4/
96	C2H4+H(+M)=C2H5(+M)	1.08E+12	0.454	1822	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.2E42 -7.62E0 6.97E3/ TROE/9.75E-1 2.1E2 9.84E2 4.374E3/
97	H2+CH3O2=H+CH3O2H	1.50E+14	0	26030	REV/1.688E18 -1.14E0 8.434E3/
98	C2H5+C2H3=2C2H4	6.86E+11	0.11	-4300	REV/4.82E14 0.0E0 7.153E4/
99	CH3+C2H5=CH4+C2H4	1.18E+04	2.45	-2921	REV/2.39E6 2.4E0 6.669E4/
100	C2H5+H=2CH3	9.69E+13	0	220	REV/2.029E9 1.028E0 1.051E4/
101	C2H5+O=CH3CHO+H	1.10E+14	0	0	REV/1.033E17 -5.0E-1 7.742E4/
102	C2H5+HO2=C2H5O+OH	1.10E+13	0	0	REV/9.68E15 -7.23E-1 2.765E4/
103	CH3O2+C2H5=CH3O+C2H5O	8.00E+12	0	-1000	REV/4.404E14 -4.25E-1 3.089E4/
104	C2H5O+O2=CH3CHO+HO2	4.28E+10	0	1097	REV/1.322E8 6.15E-1 3.413E4/
105	C2H5O=CH3+CH2O	1.32E+20	-2.018	20750	REV/3.0E11 0.0E0 6.336E3/
106	C2H5O=CH3CHO+H	5.43E+15	-0.687	22230	REV/8.0E12 0.0E0 6.4E3/
107	C2H5O2=C2H5+O2	1.31E+62	-14.784	49180	REV/2.876E56 -1.382E1 1.462E4/
108	C2H5+O2=CH3CHO+OH	8.27E+02	2.41	5285	REV/2.247E3 2.301E0 6.597E4/
109	C2H5O2=CH3CHO+OH	2.52E+41	-10.2	43710	REV/1.502E36 -9.345E0 6.984E4/
110	C2H5O2=C2H4+HO2	1.82E+38	-8.45	37890	REV/4.632E32 -7.438E0 1.67E4/
111	C2H3O1-2=CH3CO	8.50E+14	0	14000	REV/1.002E14 4.1E-2 4.871E4/
112	C2H3O1-2=CH2CHO	1.00E+14	0	14000	REV/1.245E15 -3.75E-1 4.401E4/
113	CH3CHO=CH3+HCO	7.69E+20	-1.342	86950	REV/1.75E13 0.0E0 0.0E0/
114	CH3CHO+H=CH3CO+H2	2.37E+13	0	3642	REV/1.639E10 6.33E-1 1.76E4/
115	CH3CHO+O=CH3CO+OH	5.94E+12	0	1868	REV/2.133E9 6.14E-1 1.441E4/
116	CH3CHO+OH=CH3CO+H2O	3.37E+12	0	-619	REV/2.472E10 5.27E-1 2.823E4/
117	CH3CHO+O2=CH3CO+HO2	3.01E+13	0	39150	REV/1.092E11 2.85E-1 -1.588E3/
118	CH3CHO+CH3=CH3CO+CH4	7.08E-04	4.58	1966	REV/4.468E-4 4.767E0 1.746E4/
119	CH3CHO+HO2=CH3CO+H2O2	3.01E+12	0	11920	REV/1.205E12 -6.2E-2 9.877E3/
120	CH3O2+CH3CHO=CH3O2H+CH3CO	3.01E+12	0	11920	REV/2.344E13 -5.07E-1 8.282E3/
121	CH3CHO+OH=CH2CHO+H2O	1.72E+05	2.4	815	REV/1.332E5 2.511E0 2.495E4/
122	CH3CO(+M)=CH3+CO(+M)	3.00E+12	0	16720	LOW/1.2E15 0.0E0 1.2518E4/
123	CH3CO+H=CH2CO+H2	2.00E+13	0	0	REV/1.037E13 2.01E-1 6.056E4/
124	CH3CO+O=CH2CO+OH	2.00E+13	0	0	REV/5.381E12 1.82E-1 5.914E4/
125	CH3CO+CH3=CH2CO+CH4	5.00E+13	0	0	REV/2.364E16 -2.45E-1 6.21E4/
126	CH3CO3=CH3CO+O2	6.86E+19	-1.949	38530	REV/1.2E11 0.0E0 -1.1E3/
127	CH2CHO+O2=>CH2O+CO+OH	8.95E+13	-0.6	10120	

(cont. on next page)

Table B .2. (cont.)

128	CH2+CO(+M)=CH2CO(+M)	8.10E+11	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/2.69E33 -5.11E0 7.095E3/ TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
129	CH2CO+H=HCCO+H2	2.00E+14	0	8000	REV/1.434E11 4.7E-1 4.52E3/
130	CH2CO+O=CH2+CO2	1.75E+12	0	1350	REV/2.854E9 8.09E-1 4.944E4/
131	CH2CO+O=HCCO+OH	1.00E+13	0	8000	REV/3.723E9 4.52E-1 3.108E3/
132	CH2CO+OH=HCCO+H2O	1.00E+13	0	2000	REV/7.604E10 3.65E-1 1.341E4/
133	CH2(S)+CH2CO=C2H4+CO	1.60E+14	0	0	REV/3.75E14 2.17E-1 1.034E5/
134	HCCO+OH=>H2+2CO	1.00E+14	0	0	
135	HCCO+O=>H+2CO	8.00E+13	0	0	
136	CH+CH2O=H+CH2CO	9.46E+13	0	-515	REV/1.623E15 0.0E0 6.906E4/
137	CH+HCCO=CO+C2H2	5.00E+13	0	0	REV/1.721E17 0.0E0 1.646E5/
138	C2H4(+M)=C2H2+H2(+M)	8.00E+12	0.44	88770	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/1.58E51 -9.3E0 9.78E4/ TROE/7.35E-1 1.8E2 1.035E3 5.417E3/
139	C2H4+O=CH2CHO+H	4.99E+06	1.88	183	REV/1.541E9 1.201E0 1.878E4/
140	C2H4+CH3=C2H3+CH4	6.62E+00	3.7	9500	REV/1.908E0 3.76E0 3.28E3/
141	C2H4+CH3O=C2H3+CH3OH	1.20E+11	0	6750	REV/8.138E8 2.93E-1 -7.83E2/
142	C2H4+CH3O2=C2H3+CH3O2H	2.23E+12	0	17190	REV/7.929E12 -6.34E-1 -8.167E3/
143	CH+CH4=C2H4+H	6.00E+13	0	0	REV/3.573E14 0.0E0 5.548E4/
144	CH2(S)+CH3=C2H4+H	2.00E+13	0	0	REV/6.128E19 -1.223E0 7.305E4/
145	C2H2+H(+M)=C2H3(+M)	1.71E+10	1.266	2709	Third body: H2 /2.0/ LOW/6.346E31 -4.664E0 3.78E3/ TROE/7.88E-1 -1.02E4 1.0E-30/
146	C2H3+O2=CH2O+HCO	8.50E+28	-5.312	6500	REV/3.994E27 -4.883E0 9.345E4/
147	C2H3+H=C2H2+H2	9.64E+13	0	0	REV/9.427E13 2.53E-1 6.924E4/
148	C2H3+OH=C2H2+H2O	5.00E+12	0	0	REV/5.184E13 1.47E-1 8.413E4/
149	C2H+H(+M)=C2H2(+M)	1.00E+17	0	0	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/3.75E33 -4.8E0 1.9E3/ TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
150	C2H2+O2=HCCO+OH	2.00E+08	1.5	30100	REV/2.039E6 1.541E0 3.227E4/
151	O+C2H2=C2H+OH	4.60E+19	-1.4	28950	REV/3.023E15 -6.04E-1 -1.782E3/
152	C2H2+O=HCCO+H	9.03E+12	0	4532	
153	C2H2+OH=C2H+H2O	9.00E+13	0	12950	
154	C2H2+OH=CH2CO+H	2.18E-04	4.5	-1000	
155	C2H2+OH=CH3+CO	4.83E-04	4	-2000	REV/3.495E-6 4.638E0 5.212E4/
156	OH+C2H2=H+HCCOH	5.04E+05	2.3	13500	REV/3.852E9 1.436E0 4.382E3/
157	H+HCCOH=H+CH2CO	1.00E+13	0	0	REV/9.299E13 -2.9E-1 3.111E4/
158	PC2H4OH=C2H4+OH	1.05E+25	-3.99	30390	REV/4.17E20 -2.84E0 1.24E3/
159	SC2H4OH+M=CH3CHO+H+M	1.00E+14	0	25000	REV/2.742E12 4.62E-1 -4.7E2/
160	O2C2H4OH=PC2H4OH+O2	3.90E+16	-1	30000	REV/1.2E11 0.0E0 -1.1E3/
161	O2C2H4OH=>OH+2CH2O	3.13E+09	0	18900	

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Table B .2. (cont.)

162	SC2H4OH+O2=CH3CHO+HO2	3.81E+06	2	1641	REV/2.19E5 2.39E0 2.504E4/
163	CH3COCH2=CH2CO+CH3	1.00E+14	0	31000	REV/1.0E11 0.0E0 6.0E3/
164	CH3COCH2O2=CH3COCH2+O2	2.02E+15	-0.956	24460	REV/1.2E11 0.0E0 -1.1E3/
165	CH2O+CH3COCH2O2=HCO+CH3COCH2O2H	1.29E+11	0	9000	REV/2.512E10 0.0E0 1.01E4/
166	HO2+CH3COCH2O2=>CH3COCH2O2H+O2	1.00E+12	0	0	
167	C2H3CHO=C2H3+HCO	2.00E+24	-2.135	103400	REV/1.81E13 0.0E0 0.0E0/
168	C2H3CHO+H=C2H3CO+H2	1.34E+13	0	3300	REV/3.311E10 6.13E-1 2.268E4/
169	C2H3CHO+O=C2H3CO+OH	5.94E+12	0	1868	REV/7.618E9 5.94E-1 1.984E4/
170	C2H3CHO+OH=C2H3CO+H2O	9.24E+06	1.5	-962	REV/2.42E5 2.007E0 3.331E4/
171	C2H3CHO+O2=C2H3CO+HO2	1.01E+13	0	40700	REV/1.302E11 2.65E-1 5.391E3/
172	C2H3CHO+HO2=C2H3CO+H2O2	3.01E+12	0	11920	REV/4.303E12 -8.2E-2 1.53E4/
173	C2H3CHO+CH3=C2H3CO+CH4	2.61E+06	1.78	5911	REV/5.878E6 1.947E0 2.683E4/
174	C2H3CHO+C2H3=C2H3CO+C2H4	1.74E+12	0	8440	REV/1.0E13 0.0E0 2.8E4/
175	C2H3CHO+CH3O=C2H3CO+CH3OH	1.00E+12	0	3300	REV/5.304E10 4.01E-1 2.291E4/
176	C2H3CHO+CH3O2=C2H3CO+CH3O2H	3.01E+12	0	11920	REV/8.371E13 -5.27E-1 1.371E4/
177	C2H3CO=C2H3+CO	1.37E+21	-2.179	39410	REV/1.51E11 0.0E0 4.81E3/
178	C2H5CHO=C2H5+HCO	1.50E+27	-3.205	87040	REV/1.81E13 0.0E0 0.0E0/
179	C2H5CHO+H=C2H5CO+H2	4.00E+13	0	4200	REV/2.377E10 6.54E-1 1.813E4/
180	C2H5CHO+O=C2H5CO+OH	5.00E+12	0	1790	REV/1.542E9 6.36E-1 1.431E4/
181	C2H5CHO+OH=C2H5CO+H2O	2.69E+10	0.76	-340	REV/1.695E8 1.308E0 2.848E4/
182	C2H5CHO+CH3=C2H5CO+CH4	2.61E+06	1.78	5911	REV/1.414E6 1.988E0 2.138E4/
183	C2H5CHO+HO2=C2H5CO+H2O2	2.80E+12	0	13600	REV/9.626E11 -4.1E-2 1.153E4/
184	C2H5CHO+CH3O=C2H5CO+CH3OH	1.00E+12	0	3300	REV/1.276E10 4.42E-1 1.746E4/
185	C2H5CHO+CH3O2=C2H5CO+CH3O2H	3.01E+12	0	11920	REV/2.013E13 -4.85E-1 8.26E3/
186	C2H5CHO+C2H5=C2H5CO+C2H6	1.00E+12	0	8000	REV/6.432E12 -2.8E-2 1.97E4/
187	C2H5CHO+O2=C2H5CO+HO2	1.01E+13	0	40700	REV/3.131E10 3.06E-1 -5.8E1/
188	C2H5CHO+C2H3=C2H5CO+C2H4	1.70E+12	0	8440	REV/3.198E12 1.48E-1 3.013E4/
189	C2H5CO=C2H5+CO	2.46E+23	-3.208	17550	REV/1.51E11 0.0E0 4.81E3/
190	CH3OCO=CH3+CO2	3.59E+14	-0.172	16010	REV/4.76E7 1.54E0 3.47E4/
191	CH3OCO=CH3O+CO	1.43E+15	-0.041	23770	REV/1.55E6 2.02E0 5.73E3/
192	C3H8(+M)=CH3+C2H5(+M)	1.29E+37	-5.84	97380	Third body: H2 /2.0/ Third body: H2O /6.0/ Third body: AR /0.7/ Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: CH4 /2.0/ Third body: C2H6 /3.0/ Third body: HE /0.7/ LOW/5.64E74 -1.574E1 9.8714E4/ TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
193	C3H8=NC3H7+H	3.75E+17	-0.357	101200	REV/1.0E14 0.0E0 0.0E0/
194	C3H8=IC3H7+H	2.38E+18	-0.671	98680	REV/1.0E14 0.0E0 0.0E0/
195	C3H8+O2=IC3H7+HO2	2.00E+13	0	49640	REV/1.764E9 5.99E-1 -1.69E2/
196	C3H8+O2=NC3H7+HO2	6.00E+13	0	52290	REV/3.354E10 2.85E-1 -5.9E1/
197	H+C3H8=H2+IC3H7	1.30E+06	2.4	4471	REV/2.186E1 3.347E0 9.351E3/
198	H+C3H8=H2+NC3H7	1.33E+06	2.54	6756	REV/1.418E2 3.173E0 9.096E3/
199	C3H8+O=IC3H7+OH	5.49E+05	2.5	3140	REV/4.793E0 3.428E0 6.608E3/
200	C3H8+O=NC3H7+OH	3.71E+06	2.4	5505	REV/2.053E2 3.014E0 6.433E3/
201	C3H8+OH=NC3H7+H2O	1.05E+10	0.97	1586	REV/1.191E7 1.497E0 1.882E4/
202	C3H8+OH=IC3H7+H2O	4.67E+07	1.61	-35	REV/8.327E3 2.451E0 1.974E4/
203	C3H8+HO2=IC3H7+H2O2	5.88E+04	2.5	14860	REV/5.721E2 2.752E0 3.742E3/
204	C3H8+HO2=NC3H7+H2O2	8.10E+04	2.5	16690	REV/4.995E3 2.438E0 3.03E3/

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Table B .2. (cont.)

205	CH3+C3H8=CH4+IC3H7	6.40E+04	2.17	7520	REV/9.819E2 2.671E0 1.394E4/
206	CH3+C3H8=CH4+NC3H7	9.04E-01	3.65	7154	REV/8.791E-2 3.837E0 1.103E4/
207	IC3H7+C3H8=NC3H7+C3H8	3.00E+10	0	12900	REV/3.0E10 0.0E0 1.29E4/
208	C2H3+C3H8=C2H4+IC3H7	1.00E+11	0	10400	REV/1.31E11 0.0E0 1.78E4/
209	C2H3+C3H8=C2H4+NC3H7	1.00E+11	0	10400	REV/1.31E11 0.0E0 1.78E4/
210	C2H5+C3H8=C2H6+IC3H7	1.00E+11	0	10400	REV/3.63E10 0.0E0 9.934E3/
211	C2H5+C3H8=C2H6+NC3H7	1.00E+11	0	10400	REV/3.63E10 0.0E0 9.934E3/
212	C3H8+C3H5-A=NC3H7+C3H6	7.94E+11	0	20500	REV/5.372E16 -1.33E0 1.34E4/
213	C3H8+C3H5-A=IC3H7+C3H6	7.94E+11	0	16200	REV/5.372E16 -1.33E0 9.095E3/
214	C3H8+CH3O=NC3H7+CH3OH	3.00E+11	0	7000	REV/1.22E10 0.0E0 9.182E3/
215	C3H8+CH3O=IC3H7+CH3OH	3.00E+11	0	7000	REV/1.22E10 0.0E0 9.182E3/
216	CH3O2+C3H8=CH3O2H+NC3H7	8.10E+04	2.5	16690	REV/9.718E4 1.993E0 1.435E3/
217	CH3O2+C3H8=CH3O2H+IC3H7	5.88E+04	2.5	14860	REV/1.113E4 2.307E0 2.147E3/
218	IC3H7=H+C3H6	6.92E+13	-0.025	37690	REV/2.64E13 0.0E0 2.16E3/
219	IC3H7+H=C2H5+CH3	2.00E+13	0	0	REV/4.344E7 1.176E0 8.62E3/
220	IC3H7+O2=C3H6+HO2	4.50E-19	0	5020	REV/2.0E-19 0.0E0 1.75E4/
221	IC3H7+OH=C3H6+H2O	2.41E+13	0	0	REV/2.985E12 5.7E-1 8.382E4/
222	IC3H7+O=CH3CHO+CH3	4.82E+13	0	0	REV/1.279E11 8.0E-1 8.648E4/
223	NC3H7=CH3+C2H4	9.97E+40	-8.6	41430	REV/1.898E34 -6.99E0 1.71E4/
224	NC3H7=H+C3H6	8.78E+39	-8.1	46580	REV/2.07E37 -7.39E0 1.202E4/
225	NC3H7+O2=C3H6+HO2	3.00E-19	0	3000	REV/2.0E-19 0.0E0 1.75E4/
226	C2H5CHO+NC3H7=C2H5CO+C3H8	1.70E+12	0	8440	REV/1.9E14 0.0E0 1.879E4/
227	C2H5CHO+IC3H7=C2H5CO+C3H8	1.70E+12	0	8440	REV/1.9E14 0.0E0 1.879E4/
228	C2H5CHO+C3H5-A=C2H5CO+C3H6	1.70E+12	0	8440	REV/1.0E13 0.0E0 2.8E4/
229	C3H6=C2H3+CH3	2.73E+62	-13.28	123200	REV/6.822E53 -1.1779E1 2.055E4/
230	C3H6=C3H5-A+H	2.01E+61	-13.26	118500	REV/2.041E61 -1.352E1 3.061E4/
231	C3H6=C3H5-S+H	7.71E+69	-16.09	140000	REV/2.551E67 -1.5867E1 2.869E4/
232	C3H6=C3H5-T+H	5.62E+71	-16.58	139300	REV/4.26E68 -1.6164E1 3.008E4/
233	C3H6+O=C2H5+HCO	1.58E+07	1.76	-1216	REV/9.188E1 2.725E0 2.311E4/
234	C3H6+O=>CH2CO+CH3+H	2.50E+07	1.76	76	
235	C3H6+O=>CH3CHCO+2H	2.50E+07	1.76	76	
236	C3H6+O=C3H5-A+OH	5.24E+11	0.7	5884	REV/1.104E11 6.97E-1 2.015E4/
237	C3H6+O=C3H5-S+OH	1.20E+11	0.7	8959	REV/8.239E7 1.18E0 -2.07E2/
238	C3H6+O=C3H5-T+OH	6.03E+10	0.7	7632	REV/9.483E6 1.373E0 5.76E2/
239	C3H6+OH=C3H5-A+H2O	3.12E+06	2	-298	REV/1.343E7 1.909E0 3.027E4/
240	C3H6+OH=C3H5-S+H2O	2.11E+06	2	2778	REV/2.959E4 2.393E0 9.916E3/
241	C3H6+OH=C3H5-T+H2O	1.11E+06	2	1451	REV/3.565E3 2.586E0 1.07E4/
242	C3H6+HO2=C3H5-A+H2O2	2.70E+04	2.5	12340	REV/6.341E6 1.82E0 1.201E4/
243	C3H6+HO2=C3H5-S+H2O2	1.80E+04	2.5	27620	REV/1.377E4 2.304E0 3.864E3/
244	C3H6+HO2=C3H5-T+H2O2	9.00E+03	2.5	23590	REV/1.577E3 2.497E0 1.941E3/
245	C3H6+H=C3H5-A+H2	1.73E+05	2.5	2492	REV/7.023E4 2.515E0 1.817E4/
246	C3H6+H=C3H5-S+H2	8.04E+05	2.5	12280	REV/1.063E3 2.999E0 4.526E3/
247	C3H6+H=C3H5-T+H2	4.05E+05	2.5	9794	REV/1.227E2 3.192E0 4.15E3/
248	C3H6+H=C2H4+CH3	2.30E+13	0	2547	REV/7.272E7 1.271E0 1.12E4/
249	C3H6+O2=C3H5-A+HO2	4.00E+12	0	39900	REV/8.514E12 -3.33E-1 8.87E2/
250	C3H6+O2=C3H5-S+HO2	2.00E+12	0	62900	REV/1.387E10 1.51E-1 4.59E2/
251	C3H6+O2=C3H5-T+HO2	1.40E+12	0	60700	REV/2.224E9 3.44E-1 3.69E2/
252	C3H6+CH3=C3H5-A+CH4	2.21E+00	3.5	5675	REV/8.184E2 3.07E0 2.289E4/

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Table B .2. (cont.)

253	C3H6+CH3=C3H5-S+CH4	1.35E+00	3.5	12850	REV/1.626E0 3.553E0 6.635E3/
254	C3H6+CH3=C3H5-T+CH4	8.40E-01	3.5	11660	REV/2.322E-1 3.746E0 7.552E3/
255	C3H6+C2H5=C3H5-A+C2H6	1.00E+11	0	9800	REV/5.369E5 1.33E0 1.644E4/
256	C3H6+CH3O2=C3H5-A+CH3O2H	3.24E+11	0	14900	REV/2.0E10 0.0E0 1.5E4/
257	C3H6OH=C3H6+OH	4.34E+15	-0.805	27900	REV/9.93E11 0.0E0 -9.6E2/
258	HOC3H6O2=C3H6OH+O2	2.87E+19	-1.897	34290	REV/1.2E11 0.0E0 -1.1E3/
259	HOC3H6O2=>CH3CHO+CH2O+OH	1.25E+10	0	18900	
260	C3H5-A=C2H2+CH3	2.40E+48	-9.9	82080	REV/2.61E46 -9.82E0 3.695E4/
261	C3H5-A=C3H4-A+H	4.19E+13	0.216	61930	REV/2.4E11 6.9E-1 3.007E3/
262	C3H5-A+HO2=C3H5O+OH	7.00E+12	0	-1000	REV/1.605E12 6.0E-2 1.166E4/
263	C3H5-A+CH3O2=C3H5O+CH3O	7.00E+12	0	-1000	REV/1.99E15 -7.4E-1 1.702E4/
264	C3H5-A+C2H5=C2H6+C3H4-A	4.00E+11	0	0	REV/1.802E12 5.0E-2 4.033E4/
265	C3H5-A+C2H5=C2H4+C3H6	4.00E+11	0	0	REV/6.937E16 -1.33E0 5.28E4/
266	C3H5-A+C2H3=C2H4+C3H4-A	1.00E+12	0	0	REV/1.624E13 5.0E-2 4.819E4/
267	C3H4-A+C3H6=2C3H5-A	4.75E+08	0.734	28700	REV/8.43E10 0.0E0 -2.62E2/
268	C3H5-A+O2=C3H4-A+HO2	2.18E+21	-2.85	30760	REV/2.614E19 -2.449E0 2.071E4/
269	C3H5-A+O2=CH2CHO+CH2O	7.14E+15	-1.21	21050	REV/4.944E16 -1.4E0 8.862E4/
270	C3H5-A+O2=C2H3CHO+OH	2.47E+13	-0.44	23020	REV/1.989E13 -6.09E-1 7.514E4/
271	C3H5-A+O2=>C2H2+CH2O+OH	9.72E+29	-5.71	21450	
272	C3H5-S=C2H2+CH3	9.60E+39	-8.17	42030	REV/1.61E40 -8.58E0 2.033E4/
273	C3H5-S=C3H4-P+H	4.19E+15	-0.79	37480	REV/5.8E12 0.0E0 3.1E3/
274	C3H5-S+O2=CH3CHO+HCO	4.34E+12	0	0	REV/1.611E17 -1.27E0 9.653E4/
275	C3H5-S+H=C3H4-A+H2	3.33E+12	0	0	REV/7.977E12 1.1E-1 6.886E4/
276	C3H5-S+CH3=C3H4-A+CH4	1.00E+11	0	0	REV/6.253E12 1.1E-1 6.934E4/
277	C3H5-T=C2H2+CH3	2.16E+40	-8.31	45110	REV/1.61E40 -8.58E0 2.033E4/
278	C3H5-T=C3H4-A+H	3.51E+14	-0.44	40890	REV/8.5E12 0.0E0 2.0E3/
279	C3H5-T=C3H4-P+H	1.08E+15	-0.6	38490	REV/6.5E12 0.0E0 2.0E3/
280	C3H5-T+O2=C3H4-A+HO2	1.89E+30	-5.59	15540	REV/3.037E31 -5.865E0 2.681E4/
281	C3H5-T+O2=CH3COCH2+O	3.81E+17	-1.36	5580	REV/2.0E11 0.0E0 1.75E4/
282	C3H5-T+O2=CH2O+CH3CO	3.71E+25	-3.96	7043	REV/1.872E27 -4.43E0 1.012E5/
283	C3H5-T+H=C3H4-P+H2	3.33E+12	0	0	REV/2.138E16 -8.8E-1 7.105E4/
284	C3H5-T+CH3=C3H4-P+CH4	1.00E+11	0	0	REV/1.676E16 -8.8E-1 7.153E4/
285	C3H4-A=C3H4-P	1.20E+15	0	92400	REV/3.222E18 -9.9E-1 9.659E4/
286	C3H4-A+O2=C3H3+HO2	4.00E+13	0	39160	REV/3.17E11 -8.6E-2 3.11E2/
287	C3H4-A+HO2=CH2CO+CH2+OH	4.00E+12	0	19000	REV/1.0E0 0.0E0 0.0E0/
288	C3H4-A+OH=CH2CO+CH3	3.12E+12	0	-397	REV/1.806E17 -1.38E0 3.607E4/
289	C3H4-A+O=C2H4+CO	7.80E+12	0	1600	REV/3.269E8 1.252E0 1.219E5/
290	C3H4-A+O=C2H2+CH2O	3.00E-03	4.61	-4243	REV/2.32E2 3.23E0 8.119E4/
291	C3H4-A+C3H5-A=C3H3+C3H6	2.00E+11	0	7700	REV/2.644E19 -2.71E0 4.214E4/
292	C3H4-A+C2H=C3H3+C2H2	1.00E+13	0	0	REV/1.42E16 -1.38E0 5.382E4/
293	C3H4-P+O2=HCCO+OH+CH2	1.00E+07	1.5	30100	REV/1.0E0 0.0E0 0.0E0/
294	C3H4-P+O2=C3H3+HO2	2.00E+13	0	41600	REV/6.371E11 -2.08E-1 1.021E3/
295	C3H4-P+HO2=C2H4+CO+OH	3.00E+12	0	19000	REV/1.0E0 0.0E0 0.0E0/
296	C3H4-P+OH=C3H3+H2O	1.00E+07	2	1000	REV/6.441E5 2.034E0 3.0E4/
297	C3H4-P+OH=CH2CO+CH3	5.00E-04	4.5	-1000	REV/1.079E-2 4.11E0 3.128E4/
298	C3H4-P+O=C2H3+HCO	3.20E+12	0	2010	REV/2.548E12 -3.9E-1 3.235E4/
299	C3H4-P+O=HCCO+CH3	9.60E+08	1	0	REV/1.43E4 1.793E0 2.699E4/
300	C3H4-P+O=HCCO+CH2+H	3.20E-19	0	2010	REV/1.0E-30 0.0E0 0.0E0/

(cont. on next page)

Table B .2. (cont.)

301	C3H4-P+O=C3H3+OH	7.65E+08	1.5	8600	REV/2.177E8 1.31E0 2.247E4/
302	C3H4-P+H=C3H3+H2	2.00E+07	2	5000	REV/1.215E5 2.14E0 1.911E4/
303	C3H4-P+CH3=C3H3+CH4	1.50E+00	3.5	5600	REV/8.313E0 3.195E0 2.125E4/
304	C3H4-P+C2H3=C3H3+C2H4	1.00E+12	0	7700	REV/9.541E11 -3.9E-1 5.245E4/
305	C3H4-P+C3H5-A=C3H3+C3H6	1.00E+12	0	7700	REV/4.931E16 -1.73E0 3.795E4/
306	C3H3+OH=C3H2+H2O	2.00E+13	0	8000	
307	C3H3+O2=CH2CO+HCO	3.01E+10	0	2870	REV/4.881E11 0.0E0 5.947E4/
308	C3H3+CH3=C2H5+C2H	4.30E+15	-0.79	45630	REV/1.81E13 0.0E0 0.0E0/
309	C3H2+O2=HCO+HCCO	5.00E+13	0	0	REV/2.326E14 -2.14E-1 7.719E4/
310	C3H4-A+HO2=C2H4+CO+OH	1.00E+12	0	14000	REV/1.0E0 0.0E0 0.0E0/
311	C3H4-A+HO2=C3H3+H2O2	3.00E+13	0	14000	REV/1.551E16 -1.38E0 4.4E4/
312	C2H2+CH3=C3H4-A+H	6.74E+19	-2.08	31590	REV/6.407E25 -3.345E0 2.177E4/
313	C3H3+H=C3H2+H2	2.14E+05	2.52	7453	
314	C3H2+OH=C2H2+HCO	5.00E+13	0	0	REV/2.282E16 -2.54E-1 7.502E4/
315	C3H2+O2=>HCCO+CO+H	5.00E+13	0	0	
316	CH3CHCO+OH=>C2H5+CO2	1.73E+12	0	-1010	
317	CH3CHCO+OH=>SC2H4OH+CO	2.00E+12	0	-1010	
318	CH3CHCO+H=>C2H5+CO	4.40E+12	0	1459	
319	CH3CHCO+O=>CH3CHO+CO	3.20E+12	0	-437	
320	NC3H7O2=NC3H7+O2	2.40E+20	-1.616	35960	REV/4.52E12 0.0E0 0.0E0/
321	NC3H7O2=C3H6OOH1-2	6.00E+11	0	26850	REV/1.117E8 5.83E-1 1.172E4/
322	C3H6OOH1-2=C3H6+HO2	7.83E+15	-1.3	15950	REV/1.0E11 0.0E0 1.1E4/
323	C3H6OOH1-2=>C2H4+CH2O+OH	1.31E+33	-7.01	48120	
324	C3H6OOH1-2O2=C3H6OOH1-2+O2	2.39E+25	-2.945	40100	REV/5.0E12 0.0E0 0.0E0/
325	C3H5O=C2H3CHO+H	1.00E+14	0	29100	REV/1.676E14 -1.56E-1 1.969E4/
326	C3H5O=C2H3+CH2O	1.46E+20	-1.968	35090	REV/1.5E11 0.0E0 1.06E4/
327	C3H5O+O2=C2H3CHO+HO2	1.00E+12	0	6000	REV/1.288E11 0.0E0 3.2E4/
328	NC3H7O2=C3H6+HO2	5.04E+38	-8.112	40490	REV/1.198E30 -6.229E0 2.042E4/
329	PC4H9=C2H5+C2H4	3.50E+12	0.463	29470	REV/1.32E4 2.48E0 6.13E3/
330	SC4H9=C3H6+CH3	4.80E+10	1.044	30350	REV/1.76E4 2.48E0 6.13E3/
331	PC4H9=C4H8-1+H	2.62E+12	0.253	35700	REV/2.5E11 5.1E-1 2.62E3/
332	SC4H9=C4H8-2+H	2.84E+11	0.337	35520	REV/2.5E11 5.1E-1 2.62E3/
333	SC4H9=C4H8-1+H	3.03E+11	0.591	36820	REV/4.24E11 5.1E-1 1.23E3/
334	PC4H9+O2=C4H8-1+HO2	2.00E-18	0	5000	REV/2.0E-19 0.0E0 1.75E4/
335	SC4H9+O2=C4H8-1+HO2	2.00E-18	0	5000	REV/2.0E-19 0.0E0 1.75E4/
336	SC4H9+O2=C4H8-2+HO2	2.00E-18	0	5000	REV/2.0E-19 0.0E0 1.75E4/
337	C4H8-1=C3H5-A+CH3	5.08E+19	-1.256	76510	REV/1.35E13 0.0E0 0.0E0/
338	C4H8-1=C2H3+C2H5	2.88E+23	-1.99	101600	REV/9.0E12 0.0E0 0.0E0/
339	C4H8-1=H+C4H71-3	3.72E+14	-0.111	85200	REV/5.0E13 0.0E0 0.0E0/
340	C4H8-1+O2=C4H71-3+HO2	2.00E+13	0	37190	REV/4.653E12 7.0E-2 -1.68E2/
341	C4H8-1+H=C4H71-2+H2	3.90E+05	2.5	5821	REV/2.558E4 2.55E0 2.125E3/
342	C4H8-1+H=C4H71-3+H2	3.38E+05	2.36	207	REV/4.323E6 2.1E0 2.033E4/
343	C4H8-1+H=C4H71-4+H2	6.65E+05	2.54	6756	REV/3.045E4 2.54E0 1.103E4/
344	C4H8-1+OH=C4H71-2+H2O	2.22E+06	2	1451	REV/6.304E5 2.05E0 1.291E4/
345	C4H8-1+OH=C4H71-3+H2O	2.76E+04	2.64	-1919	REV/1.532E6 2.38E0 3.336E4/
346	C4H8-1+OH=C4H71-4+H2O	5.27E+09	0.97	1586	REV/1.044E9 9.7E-1 2.101E4/
347	C4H8-1+CH3=C4H71-3+CH4	3.69E+00	3.31	4002	REV/1.234E3 3.05E0 2.461E4/
348	C4H8-1+CH3=C4H71-4+CH4	4.52E-01	3.65	7154	REV/5.405E-1 3.65E0 1.191E4/

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Table B .2. (cont.)

349	C4H8-1+HO2=C4H71-3+H2O2	4.82E+03	2.55	10530	REV/1.586E6 1.96E0 1.435E4/
350	C4H8-1+HO2=C4H71-4+H2O2	2.38E+03	2.55	16490	REV/2.8E3 2.22E0 4.46E3/
351	C4H8-1+CH3O2=C4H71-3+CH3O2H	4.82E+03	2.55	10530	REV/3.303E6 1.79E0 1.133E4/
352	C4H8-1+CH3O2=C4H71-4+CH3O2H	2.38E+03	2.55	16490	REV/5.831E3 2.04E0 1.44E3/
353	C4H8-1+CH3O=C4H71-3+CH3OH	4.00E+01	2.9	8609	REV/2.47E2 2.67E0 2.7E4/
354	C4H8-1+CH3O=C4H71-4+CH3OH	2.17E+11	0	6458	REV/4.789E9 2.0E-2 9.002E3/
355	C4H8-1+C3H5-A=C4H71-3+C3H6	7.90E+10	0	12400	REV/1.0E11 0.0E0 1.75E4/
356	C4H8-1+C4H6=2C4H71-3	2.35E+12	0	46720	REV/1.6E12 0.0E0 0.0E0/
357	C4H8-2=H+C4H71-3	2.34E+14	0.143	87890	REV/5.0E13 0.0E0 0.0E0/
358	C4H8-2+O2=C4H71-3+HO2	4.00E+13	0	39390	REV/1.35E13 -1.8E-1 -9.24E2/
359	C4H8-2+H=C4H71-3+H2	3.46E+05	2.5	2492	REV/6.428E6 1.99E0 1.966E4/
360	C4H8-2+OH=C4H71-3+H2O	6.24E+06	2	-298	REV/5.019E8 1.49E0 3.202E4/
361	C4H8-2+CH3=C4H71-3+CH4	4.42E+00	3.5	5675	REV/2.145E3 2.99E0 2.332E4/
362	C4H8-2+HO2=C4H71-3+H2O2	1.93E+04	2.6	13910	REV/9.205E6 1.77E0 1.477E4/
363	C4H8-2+CH3O2=C4H71-3+CH3O2H	1.93E+04	2.6	13910	REV/1.917E7 1.59E0 1.175E4/
364	C4H8-2+CH3O=C4H71-3+CH3OH	1.80E+01	2.95	11990	REV/1.612E2 2.47E0 2.742E4/
365	PC4H8OH=C4H8-1+OH	1.08E+16	-0.699	28090	REV/4.75E12 0.0E0 -7.82E2/
366	C4H8OH-1O2=PC4H8OH+O2	6.75E+20	-1.944	35520	REV/2.0E12 0.0E0 0.0E0/
367	C4H8OH-1O2=>C2H5CHO+CH2O+OH	1.00E+16	0	25000	
368	C4H71-2=C3H4-A+CH3	9.59E+14	-0.71	31260	REV/2.0E11 0.0E0 7.8E3/
369	C4H71-4=C2H4+C2H3	8.77E+12	-0.22	36290	REV/2.0E11 0.0E0 7.8E3/
370	C4H71-3=C4H6+H	1.20E+14	0	49300	REV/4.0E13 0.0E0 1.3E3/
371	C4H71-3+C2H5=C4H8-1+C2H4	2.59E+12	0	-131	REV/1.149E13 6.0E-2 4.944E4/
372	C4H71-3+CH3O=C4H8-1+CH2O	2.41E+13	0	0	REV/2.482E12 2.8E-1 6.633E4/
373	C4H71-3+O=C2H3CHO+CH3	6.03E+13	0	0	REV/3.385E15 -7.8E-1 8.163E4/
374	C4H71-3+HO2=C4H7O+OH	9.64E+12	0	0	REV/7.29E15 -1.09E0 1.553E4/
375	C4H71-3+CH3O2=C4H7O+CH3O	9.64E+12	0	0	REV/7.12E17 -1.67E0 2.029E4/
376	C3H5-A+C4H71-3=C3H6+C4H6	6.31E+12	0	0	REV/1.0E10 0.0E0 5.0E4/
377	C4H71-3+O2=C4H6+HO2	1.00E+09	0	0	REV/1.0E11 0.0E0 1.7E4/
378	H+C4H71-3=C4H6+H2	3.16E+13	0	0	REV/1.066E13 0.0E0 5.681E4/
379	C2H5+C4H71-3=C4H6+C2H6	3.98E+12	0	0	REV/3.211E12 0.0E0 4.984E4/
380	C2H3+C4H71-3=C2H4+C4H6	3.98E+12	0	0	REV/1.157E13 0.0E0 5.771E4/
381	C4H71-3+C2H5O2=C4H7O+C2H5O	3.80E+12	0	-1200	REV/2.0E10 0.0E0 0.0E0/
382	C4H7O=CH3CHO+C2H3	7.94E+14	0	19000	REV/1.0E10 0.0E0 2.0E4/
383	C4H7O=C2H3CHO+CH3	7.94E+14	0	19000	REV/1.0E10 0.0E0 2.0E4/
384	C4H6+OH=C2H5+CH2CO	1.00E+12	0	0	REV/3.73E12 0.0E0 3.002E4/
385	C4H6+OH=CH2O+C3H5-A	1.00E+12	0	0	REV/3.501E6 0.0E0 7.106E4/
386	C4H6+OH=C2H3+CH3CHO	1.00E+12	0	0	REV/5.437E11 0.0E0 1.855E4/
387	C4H6+O=C2H4+CH2CO	1.00E+12	0	0	REV/6.377E11 0.0E0 9.434E4/
388	C4H6+O=CH2O+C3H4-A	1.00E+12	0	0	REV/1.075E12 0.0E0 7.905E4/
389	C4H8O1-3+OH=>CH2O+C3H5-A+H2O	5.00E+12	0	0	
390	C4H8O1-3+H=>CH2O+C3H5-A+H2	5.00E+12	0	0	
391	C4H8O1-3+O=>CH2O+C3H5-A+OH	5.00E+12	0	0	
392	C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2	1.00E+13	0	15000	
393	C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.00E+13	0	19000	
394	C4H8O1-3+CH3=>CH2O+C3H5-A+CH4	2.00E+11	0	10000	
395	PC4H9O2=PC4H9+O2	2.85E+20	-1.642	35930	REV/4.52E12 0.0E0 0.0E0/
396	SC4H9O2=SC4H9+O2	4.33E+22	-2.216	38160	REV/7.54E12 0.0E0 0.0E0/

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Table B .2. (cont.)

397	PC4H9O2=C4H8OOH1-3	2.50E+10	0	20850	REV/3.231E9 -1.36E-1 7.871E3/
398	SC4H9O2=C4H8OOH2-3	2.00E+11	0	26850	REV/3.994E10 -1.96E-1 1.393E4/
399	PC4H9O2=C4H8-1+HO2	5.04E+38	-8.11	40490	REV/1.599E30 -6.283E0 2.035E4/
400	SC4H9O2=C4H8-1+HO2	5.08E+42	-9.41	41490	REV/2.595E33 -7.347E0 1.661E4/
401	SC4H9O2=C4H8-2+HO2	5.04E+38	-8.11	40490	REV/1.618E29 -5.793E0 1.83E4/
402	C4H8OOH2-3=C4H8-2+HO2	6.22E+19	-2.513	21020	REV/1.0E11 0.0E0 1.175E4/
403	C4H8OOH1-3=>C4H8O1-3+OH	7.50E+10	0	15250	
404	C4H8OOH1-3=>OH+CH2O+C3H6	6.64E+13	-0.16	29900	
405	C4H8OOH1-3O2=C4H8OOH1-3+O2	5.60E+22	-2.234	37960	REV/7.54E12 0.0E0 0.0E0/
406	C4H8OOH1-3O2=NC4KET13+OH	2.50E+10	0	21400	REV/1.435E3 1.486E0 4.474E4/
407	NC4KET13=>CH3CHO+CH2CHO+OH	1.05E+16	0	41600	
408	C2H5COCH2=CH2CO+C2H5	1.00E+14	0	35000	REV/1.0E11 0.0E0 0.0E0/
409	NC3H7CHO+O2=NC3H7CO+HO2	1.20E+05	2.5	37560	REV/1.0E7 5.0E-1 4.0E3/
410	NC3H7CHO+OH=NC3H7CO+H2O	2.00E+06	1.8	-1300	REV/1.553E4 2.32E0 2.805E4/
411	NC3H7CHO+H=NC3H7CO+H2	4.14E+09	1.12	2320	REV/3.03E6 1.746E0 1.678E4/
412	NC3H7CHO+O=NC3H7CO+OH	5.94E+12	0	1868	REV/2.258E9 6.07E-1 1.492E4/
413	NC3H7CHO+HO2=NC3H7CO+H2O2	4.09E+04	2.5	10200	REV/1.733E4 2.431E0 8.662E3/
414	NC3H7CHO+CH3=NC3H7CO+CH4	2.89E-03	4.62	3210	REV/1.93E-3 4.8E0 1.921E4/
415	NC3H7CHO+CH3O=NC3H7CO+CH3OH	1.00E+12	0	3300	REV/1.572E10 4.13E-1 1.799E4/
416	NC3H7CHO+CH3O2=NC3H7CO+CH3O2H	4.09E+04	2.5	10200	REV/3.371E5 1.986E0 7.067E3/
417	NC3H7CO=NC3H7+CO	1.00E+11	0	9600	REV/2.193E3 1.763E0 -1.1E3/
418	SC3H5CHO+OH=SC3H5CO+H2O	2.69E+10	0.76	-340	REV/4.831E10 7.7E-1 3.709E4/
419	SC3H5CO=C3H5-S+CO	8.60E+15	0	23000	REV/1.0E11 0.0E0 6.0E3/
420	SC3H5CHO+HO2=SC3H5CO+H2O2	1.00E+12	0	11920	REV/1.066E13 -3.2E-1 1.789E4/
421	SC3H5CHO+CH3=SC3H5CO+CH4	3.98E+12	0	8700	REV/4.313E13 1.0E-2 3.146E4/
422	SC3H5CHO+O=SC3H5CO+OH	7.18E+12	0	1389	REV/1.308E12 1.0E-2 2.157E4/
423	SC3H5CHO+O2=SC3H5CO+HO2	4.00E+13	0	37600	REV/3.014E11 3.4E-1 2.394E3/
424	SC3H5CHO+H=SC3H5CO+H2	2.60E+12	0	2600	REV/1.079E12 1.0E-2 2.488E4/
425	C5H11-1=C2H4+NC3H7	3.21E+12	0.451	29430	REV/8.8E3 2.48E0 6.13E3/
426	C5H11-1=H+C5H10-1	3.35E+11	0.608	35640	REV/2.5E11 5.1E-1 2.62E3/
427	C5H11-1=C5H11-2	3.88E+09	0.353	19760	REV/1.602E8 7.56E-1 2.22E4/
428	C5H11-2=C3H6+C2H5	1.22E+12	0.635	29360	REV/8.8E3 2.48E0 6.13E3/
429	C5H11-2=C5H10-1+H	2.35E+10	1.011	36680	REV/4.24E11 5.1E-1 1.23E3/
430	C5H11-2=C5H10-2+H	3.99E+11	0.41	35220	REV/2.5E11 5.1E-1 2.62E3/
431	C5H10-1=C2H5+C3H5-A	9.86E+21	-2.086	75060	REV/4.0E12 0.0E0 -5.96E2/
432	C5H10-1+H=C5H91-3+H2	3.38E+05	2.36	207	REV/3.096E5 2.53E0 2.032E4/
433	C5H10-1+H=C5H91-4+H2	1.30E+06	2.4	4471	REV/2.777E2 3.17E0 1.124E4/
434	C5H10-1+H=C5H91-5+H2	6.65E+05	2.54	6756	REV/2.193E3 2.96E0 1.102E4/
435	C5H10-1+O=C5H91-3+OH	6.60E+05	2.43	1210	REV/2.658E5 2.6E0 1.923E4/
436	C5H10-1+O=C5H91-4+OH	5.51E+05	2.45	2830	REV/5.169E1 3.22E0 7.505E3/
437	C5H10-1+O=C5H91-5+OH	9.80E+05	2.43	4750	REV/1.419E3 2.85E0 6.915E3/
438	C5H10-1+OH=C5H91-3+H2O	2.76E+04	2.64	-1919	REV/1.097E5 2.81E0 3.335E4/
439	C5H10-1+OH=C5H91-4+H2O	4.67E+07	1.61	-35	REV/4.319E4 2.38E0 2.189E4/
440	C5H10-1+OH=C5H91-5+H2O	5.27E+09	0.97	1586	REV/7.524E7 1.39E0 2.1E4/
441	C5H10-1+CH3=C5H91-3+CH4	3.69E+00	3.31	4002	REV/8.84E1 3.48E0 2.459E4/
442	C5H10-1+CH3=C5H91-4+CH4	1.51E+00	3.46	5481	REV/8.426E-3 4.23E0 1.273E4/
443	C5H10-1+CH3=C5H91-5+CH4	4.52E-01	3.65	7154	REV/3.895E-2 4.07E0 1.189E4/
444	C5H10-1+O2=C5H91-3+HO2	2.20E+12	0	37220	REV/3.665E10 4.9E-1 -1.52E2/

(cont. on next page)

Table B .2. (cont.)

445	C5H10-1+O2=C5H91-4+HO2	2.00E+13	0	49640	REV/7.76E7 1.09E0 -1.072E3/
446	C5H10-1+O2=C5H91-5+HO2	3.00E+13	0	52290	REV/1.797E9 7.5E-1 -9.32E2/
447	C5H10-1+HO2=C5H91-3+H2O2	4.82E+03	2.55	10530	REV/1.136E5 2.39E0 1.433E4/
448	C5H10-1+HO2=C5H91-4+H2O2	9.64E+03	2.6	13910	REV/5.292E1 3.04E0 4.372E3/
449	C5H10-1+HO2=C5H91-5+H2O2	2.38E+04	2.55	16490	REV/2.017E3 2.64E0 4.446E3/
450	C5H10-1+CH3O2=C5H91-3+CH3O2H	4.82E+03	2.55	10530	REV/2.366E5 2.21E0 1.131E4/
451	C5H10-1+CH3O2=C5H91-4+CH3O2H	9.64E+03	2.6	13910	REV/1.102E2 2.86E0 1.352E3/
452	C5H10-1+CH3O2=C5H91-5+CH3O2H	2.38E+04	2.55	16490	REV/4.2E3 2.47E0 1.426E3/
453	C5H10-1+CH3O=C5H91-3+CH3OH	4.00E+01	2.9	8609	REV/1.769E1 3.09E0 2.699E4/
454	C5H10-1+CH3O=C5H91-4+CH3OH	1.45E+11	0	4571	REV/1.493E7 7.9E-1 9.611E3/
455	C5H10-1+CH3O=C5H91-5+CH3OH	2.17E+11	0	6458	REV/3.45E8 4.5E-1 8.988E3/
456	C5H10-2+H=C5H91-3+H2	1.73E+05	2.5	2492	REV/4.561E6 2.06E0 1.975E4/
457	C5H10-2+H=C5H92-4+H2	3.38E+05	2.36	207	REV/4.361E6 2.1E0 2.033E4/
458	C5H10-2+H=C5H92-5+H2	6.65E+05	2.54	6756	REV/3.085E4 2.54E0 1.103E4/
459	C5H10-2+O=C5H91-3+OH	4.41E+05	2.42	3150	REV/5.107E6 1.98E0 1.831E4/
460	C5H10-2+O=C5H92-4+OH	9.90E+05	2.43	1210	REV/5.617E6 2.17E0 1.924E4/
461	C5H10-2+O=C5H92-5+OH	9.80E+05	2.43	4750	REV/1.996E4 2.42E0 6.931E3/
462	C5H10-2+OH=C5H91-3+H2O	3.12E+06	2	-298	REV/3.562E8 1.56E0 3.211E4/
463	C5H10-2+OH=C5H92-4+H2O	2.76E+04	2.64	-1919	REV/1.546E6 2.38E0 3.336E4/
464	C5H10-2+OH=C5H92-5+H2O	5.27E+09	0.97	1586	REV/1.058E9 9.6E-1 2.102E4/
465	C5H10-2+CH3=C5H91-3+CH4	2.21E+00	3.5	5675	REV/1.522E3 3.06E0 2.341E4/
466	C5H10-2+CH3=C5H92-4+CH4	3.69E+00	3.31	4002	REV/1.245E3 3.05E0 2.461E4/
467	C5H10-2+CH3=C5H92-5+CH4	4.52E-01	3.65	7154	REV/5.478E-1 3.64E0 1.191E4/
468	C5H10-2+O2=C5H91-3+HO2	3.30E+12	0	39900	REV/1.581E12 -1.1E-1 -3.26E2/
469	C5H10-2+O2=C5H92-4+HO2	2.20E+12	0	37220	REV/5.163E11 7.0E-2 -1.36E2/
470	C5H10-2+O2=C5H92-5+HO2	3.00E+13	0	52290	REV/2.528E10 3.2E-1 -9.16E2/
471	C5H10-2+HO2=C5H91-3+H2O2	9.64E+03	2.6	13910	REV/6.532E6 1.84E0 1.486E4/
472	C5H10-2+HO2=C5H92-4+H2O2	4.82E+03	2.55	10530	REV/1.6E6 1.96E0 1.435E4/
473	C5H10-2+HO2=C5H92-5+H2O2	2.38E+04	2.55	16490	REV/2.837E4 2.22E0 4.462E3/
474	C5H10-2+CH3O2=C5H91-3+CH3O2H	9.64E+03	2.6	13910	REV/1.36E7 1.66E0 1.184E4/
475	C5H10-2+CH3O2=C5H92-4+CH3O2H	4.82E+03	2.55	10530	REV/3.332E6 1.79E0 1.133E4/
476	C5H10-2+CH3O2=C5H92-5+CH3O2H	2.38E+04	2.55	16490	REV/5.908E4 2.04E0 1.442E3/
477	C5H10-2+CH3O=C5H91-3+CH3OH	9.00E+01	2.95	11990	REV/1.144E3 2.54E0 2.751E4/
478	C5H10-2+CH3O=C5H92-4+CH3OH	4.00E+01	2.9	8609	REV/2.491E2 2.67E0 2.701E4/
479	C5H10-2+CH3O=C5H92-5+CH3OH	2.17E+11	0	6458	REV/4.853E9 2.0E-2 9.004E3/
480	C5H91-3+HO2=C5H9O1-3+OH	9.64E+12	0	0	REV/6.088E15 -1.07E0 1.572E4/
481	C5H91-3+CH3O2=C5H9O1-3+CH3O	9.64E+12	0	0	REV/5.946E17 -1.65E0 2.048E4/
482	C5H91-3+C2H5O2=C5H9O1-3+C2H5O	9.64E+12	0	0	REV/3.893E14 -7.2E-1 1.833E4/
483	C5H92-4+HO2=C5H9O2-4+OH	9.64E+12	0	0	REV/7.027E15 -1.24E0 1.589E4/
484	C5H92-4+CH3O2=C5H9O2-4+CH3O	9.64E+12	0	0	REV/6.863E17 -1.82E0 2.065E4/
485	C5H92-4+C2H5O2=C5H9O2-4+C2H5O	9.64E+12	0	0	REV/4.493E14 -8.9E-1 1.849E4/
486	C5H91-3=C4H6+CH3	7.55E+14	-0.52	38520	REV/1.0E11 0.0E0 7.8E3/
487	C5H91-3=C5H81-3+H	4.73E+11	0.636	42640	REV/2.5E11 5.1E-1 2.62E3/
488	C5H91-4=C3H6+C2H3	5.81E+11	0.17	35850	REV/1.0E11 0.0E0 7.8E3/
489	C5H91-5=C2H4+C3H5-A	7.16E+16	-1.42	17750	REV/1.0E11 0.0E0 7.8E3/
490	C5H92-4=C5H81-3+H	2.02E+15	-0.34	46030	REV/1.0E13 0.0E0 1.2E3/
491	C5H92-5=C2H4+C3H5-S	8.90E+16	-1.18	42180	REV/2.0E11 0.0E0 7.8E3/
492	C5H9O1-3=C2H3CHO+C2H5	3.13E+19	-1.85	10670	REV/1.0E11 0.0E0 9.6E3/

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Table B .2. (cont.)

493	C5H9O1-3=C2H5CHO+C2H3	1.42E+18	-1.56	23340	REV/1.0E11 0.0E0 9.6E3/
494	C5H81-3+OH=CH2O+C4H71-3	1.00E+12	0	0	REV/1.0E11 0.0E0 1.5E4/
495	C5H81-3+OH=C2H3CHO+C2H5	1.00E+12	0	0	REV/1.0E11 0.0E0 1.5E4/
496	C5H81-3+OH=CH3CHO+C3H5-S	1.00E+12	0	0	REV/1.0E11 0.0E0 1.5E4/
497	C5H9O2-4=SC3H5CHO+CH3	5.98E+15	-1.13	9941	REV/1.0E11 0.0E0 9.6E3/
498	C5H9O2-4=CH3CHO+C3H5-S	1.07E+22	-2.66	29650	REV/1.0E11 0.0E0 9.6E3/
499	C5H10-2=CH3+C4H71-3	6.49E+19	-1.367	76320	REV/8.0E12 0.0E0 -5.96E2/
500	C5H11-1+O2=C5H10-1+HO2	8.37E-01	3.59	11960	REV/1.307E0 3.42E0 2.781E4/
501	C5H11-2+O2=C5H10-1+HO2	5.35E-01	3.71	9322	REV/2.021E1 3.137E0 2.274E4/
502	C5H11-2+O2=C5H10-2+HO2	1.07E+00	3.71	9322	REV/1.406E0 3.738E0 2.559E4/
503	C5H10OH-1=C5H10-1+OH	1.50E+13	0	25830	REV/4.75E12 0.0E0 -7.82E2/
504	O2C5H10OH-1=C5H10OH-1+O2	1.06E+21	-1.84	37750	REV/2.0E12 0.0E0 0.0E0/
505	O2C5H10OH-1=>NC3H7CHO+CH2O+OH	2.50E+10	0	18860	
506	C6H13-1+O2=C6H12-1+HO2	3.00E-19	0	3000	REV/2.0E-19 0.0E0 1.75E4/
507	C6H13-1=C2H4+PC4H9	6.39E+19	-1.97	30640	REV/3.3E11 0.0E0 7.2E3/
508	C6H13-1=C6H12-1+H	9.62E+13	-0.26	36000	REV/1.0E13 0.0E0 2.9E3/
509	C6H12-1=NC3H7+C3H5-A	1.00E+16	0	71000	REV/1.0E13 0.0E0 0.0E0/
510	C6H12-1+OH=>C5H11-1+CH2O	1.00E+11	0	-4000	
511	C6H12-1+O=>C5H11-1+HCO	1.00E+11	0	-1050	
512	C6H12-1+H=C6H111-3+H2	3.38E+05	2.36	207	REV/4.378E6 2.1E0 2.033E4/
513	C6H12-1+H=C6H111-6+H2	6.65E+05	2.54	6756	REV/3.12E4 2.54E0 1.103E4/
514	C6H12-1+OH=C6H111-3+H2O	2.76E+04	2.64	-1919	REV/1.552E6 2.38E0 3.336E4/
515	C6H12-1+OH=C6H111-6+H2O	5.27E+09	0.97	1586	REV/1.071E9 9.7E-1 2.101E4/
516	C6H12-1+CH3=C6H111-3+CH4	3.69E+00	3.31	4002	REV/1.25E3 3.05E0 2.46E4/
517	C6H12-1+CH3=C6H111-6+CH4	4.52E-01	3.65	7154	REV/5.541E-1 3.65E0 1.19E4/
518	C6H12-1+HO2=C6H111-3+H2O2	9.64E+03	2.55	10530	
519	C6H12-1+HO2=C6H111-6+H2O2	2.38E+04	2.55	16490	
520	C6H12-1+CH3O2=C6H111-3+CH3O2H	4.82E+03	2.55	10530	REV/3.345E6 1.79E0 1.132E4/
521	C6H12-1+CH3O2=C6H111-6+CH3O2H	2.38E+04	2.55	16490	REV/5.976E4 2.04E0 1.436E3/
522	C6H12-1+CH3O=C6H111-3+CH3OH	4.00E+01	2.9	8609	REV/2.501E2 2.67E0 2.7E4/
523	C6H12-1+CH3O=C6H111-6+CH3OH	2.17E+11	0	6458	REV/4.908E9 2.0E-2 8.998E3/
524	C6H111-3+HO2=C6H11O1-3+OH	9.64E+12	0	0	REV/1.07E16 -1.14E0 1.58E4/
525	C6H111-3+CH3O2=C6H11O1-3+CH3O	9.64E+12	0	0	REV/1.045E18 -1.72E0 2.057E4/
526	C6H111-3+C2H5O2=C6H11O1-3+C2H5O	9.64E+12	0	0	REV/6.844E14 -8.0E-1 1.841E4/
527	C6H111-6=C6H111-3	1.11E+12	0	31700	REV/3.076E14 -2.5E-1 4.755E4/
528	C6H11O1-3=C2H3CHO+NC3H7	1.43E+20	-2.04	11230	REV/1.0E11 0.0E0 9.6E3/
529	C6H11O1-3=NC3H7CHO+C2H3	2.40E+18	-1.63	23410	REV/1.0E11 0.0E0 9.6E3/
530	C6H12-1+OH=C6H12OH-1	1.00E+13	0	0	
531	C6H12OH-1+O2=O2C6H12OH-1	6.00E+12	0	0	
532	O2C6H12OH-1=NC4H9CHO+CH2O+OH	1.00E+12	0	27800	
533	NC4H9CHO+O2=NC4H9CO+HO2	2.00E+13	0.5	42200	REV/1.0E7 0.0E0 4.0E4/
534	NC4H9CHO+OH=NC4H9CO+H2O	2.69E+10	0.76	-340	REV/2.143E10 7.3E-1 3.124E4/
535	NC4H9CHO+H=NC4H9CO+H2	4.00E+13	0	4200	REV/1.8E13 0.0E0 2.4E4/
536	NC4H9CHO+O=NC4H9CO+OH	5.00E+12	0	1790	REV/1.0E12 0.0E0 1.9E4/
537	NC4H9CHO+HO2=NC4H9CO+H2O2	2.80E+12	0	13600	REV/1.0E12 0.0E0 1.0E4/
538	NC4H9CHO+CH3=NC4H9CO+CH4	1.70E+12	0	8440	REV/1.5E13 0.0E0 2.8E4/
539	NC4H9CHO+CH3O=NC4H9CO+CH3OH	1.15E+11	0	1280	REV/3.0E11 0.0E0 1.8E4/
540	NC4H9CHO+CH3O2=NC4H9CO+CH3O2H	1.00E+12	0	9500	REV/2.5E10 0.0E0 1.0E4/

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Table B .2. (cont.)

541	NC4H9CO=PC4H9+CO	1.00E+11	0	9600	REV/1.0E11 0.0E0 0.0E0/
542	NC3H7COCH2=NC3H7+CH2CO	1.23E+18	-1.4	43450	REV/1.0E11 0.0E0 1.16E4/
543	NC7H16=H+C7H15-1	2.68E+88	-21.17	142800	REV/7.264E84 -2.081E1 4.156E4/
544	NC7H16=H+C7H15-2	1.30E+88	-21.01	139500	REV/2.263E83 -2.031E1 4.083E4/
545	NC7H16=H+C7H15-3	1.30E+88	-21.01	139500	REV/2.263E83 -2.031E1 4.083E4/
546	NC7H16=H+C7H15-4	6.50E+87	-21.01	139500	REV/2.255E83 -2.031E1 4.083E4/
547	NC7H16(+M)=C6H13-1+CH3(+M)	4.33E+24	-2.12	89900	LOW/4.963E42 -7.78E0 4.28E4/ TROE/8.92E-1 1.0E10 2.228E0 1.798E9/
548	NC7H16(+M)=C5H11-1+C2H5(+M)	6.82E+26	-2.7	88910	LOW/3.753E48 -9.46E0 4.131E4/ TROE/9.0E-2 3.6556E0 1.0E10 9.33E9/
549	NC7H16(+M)=PC4H9+NC3H7(+M)	1.36E+26	-2.53	88760	LOW/6.509E48 -9.57E0 4.129E4/ TROE/9.11E-1 1.0E10 2.2382E1 5.0E9/
550	NC7H16+H=C7H15-1+H2	1.88E+05	2.75	6280	REV/2.037E1 3.38E0 8.618E3/
551	NC7H16+H=C7H15-2+H2	2.60E+06	2.4	4471	REV/1.807E1 3.38E0 9.318E3/
552	NC7H16+H=C7H15-3+H2	2.60E+06	2.4	4471	REV/1.807E1 3.38E0 9.318E3/
553	NC7H16+H=C7H15-4+H2	1.30E+06	2.4	4471	REV/1.8E1 3.38E0 9.318E3/
554	NC7H16+O=C7H15-1+OH	1.93E+05	2.68	3716	REV/1.085E1 3.29E0 4.642E3/
555	NC7H16+O=C7H15-2+OH	9.54E+04	2.71	2106	REV/3.481E-1 3.67E0 5.541E3/
556	NC7H16+O=C7H15-3+OH	9.54E+04	2.71	2106	REV/3.481E-1 3.67E0 5.541E3/
557	NC7H16+O=C7H15-4+OH	4.77E+04	2.71	2106	REV/3.468E-1 3.67E0 5.541E3/
558	NC7H16+OH=C7H15-1+H2O	2.57E+07	1.8	954	REV/2.952E4 2.33E0 1.818E4/
559	NC7H16+OH=C7H15-2+H2O	4.90E+06	2	-596	REV/3.624E2 2.87E0 1.914E4/
560	NC7H16+OH=C7H15-3+H2O	4.90E+06	2	-596	REV/3.624E2 2.87E0 1.914E4/
561	NC7H16+OH=C7H15-4+H2O	2.45E+06	2	-596	REV/3.61E2 2.87E0 1.914E4/
562	NC7H16+HO2=C7H15-1+H2O2	4.08E+01	3.59	17160	REV/2.557E0 3.53E0 3.498E3/
563	NC7H16+HO2=C7H15-2+H2O2	1.26E+02	3.37	13720	REV/4.982E-1 3.66E0 2.562E3/
564	NC7H16+HO2=C7H15-3+H2O2	1.26E+02	3.37	13720	REV/4.982E-1 3.66E0 2.562E3/
565	NC7H16+HO2=C7H15-4+H2O2	6.32E+01	3.37	13720	REV/4.952E-1 3.66E0 2.562E3/
566	NC7H16+CH3=C7H15-1+CH4	9.04E-01	3.65	7154	REV/8.935E-2 3.84E0 1.103E4/
567	NC7H16+CH3=C7H15-2+CH4	5.41E+04	2.26	7287	REV/3.432E2 2.79E0 1.367E4/
568	NC7H16+CH3=C7H15-3+CH4	5.41E+04	2.26	7287	REV/3.432E2 2.79E0 1.367E4/
569	NC7H16+CH3=C7H15-4+CH4	2.71E+04	2.26	7287	REV/3.419E2 2.79E0 1.367E4/
570	NC7H16+O2=C7H15-1+HO2	4.20E+13	0	52800	REV/2.386E10 2.8E-1 4.53E2/
571	NC7H16+O2=C7H15-2+HO2	2.80E+13	0	50150	REV/1.0E9 6.3E-1 3.09E2/
572	NC7H16+O2=C7H15-3+HO2	2.80E+13	0	50150	REV/1.0E9 6.3E-1 3.09E2/
573	NC7H16+O2=C7H15-4+HO2	1.40E+13	0	50150	REV/9.941E8 6.3E-1 3.09E2/
574	NC7H16+C2H5=C7H15-1+C2H6	1.00E+11	0	13400	REV/3.2E11 0.0E0 1.23E4/
575	NC7H16+C2H5=C7H15-2+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
576	NC7H16+C2H5=C7H15-3+C2H6	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.29E4/
577	NC7H16+C2H5=C7H15-4+C2H6	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.29E4/
578	NC7H16+CH3O=C7H15-1+CH3OH	3.16E+11	0	7000	REV/1.2E10 0.0E0 9.2E3/
579	NC7H16+CH3O=C7H15-2+CH3OH	2.19E+11	0	5000	REV/8.9E9 0.0E0 7.2E3/
580	NC7H16+CH3O=C7H15-3+CH3OH	2.19E+11	0	5000	REV/8.9E9 0.0E0 7.2E3/
581	NC7H16+CH3O=C7H15-4+CH3OH	1.10E+11	0	5000	REV/8.9E9 0.0E0 7.2E3/
582	NC7H16+C2H3=C7H15-1+C2H4	1.00E+12	0	18000	REV/2.57E12 0.0E0 2.54E4/
583	NC7H16+C2H3=C7H15-2+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
584	NC7H16+C2H3=C7H15-3+C2H4	8.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/
585	NC7H16+C2H3=C7H15-4+C2H4	4.00E+11	0	16800	REV/2.0E12 0.0E0 2.42E4/

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Table B .2. (cont.)

586	NC7H16+CH3O2=C7H15-1+CH3O2H	1.39E+00	3.97	18280	REV/1.69E0 3.46E0 3.024E3/
587	NC7H16+CH3O2=C7H15-2+CH3O2H	2.04E+01	3.58	14810	REV/1.562E0 3.42E0 2.054E3/
588	NC7H16+CH3O2=C7H15-3+CH3O2H	2.04E+01	3.58	14810	REV/1.562E0 3.42E0 2.054E3/
589	NC7H16+CH3O2=C7H15-4+CH3O2H	1.02E+01	3.58	14810	REV/1.553E0 3.42E0 2.054E3/
590	NC7H16+C7H15O2-3=C7H15-1+C7H15O2H-3	1.21E+13	0	20430	REV/1.44E10 0.0E0 1.5E4/
591	NC7H16+C7H15O2-3=C7H15-2+C7H15O2H-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
592	NC7H16+C7H15O2-3=C7H15-3+C7H15O2H-3	8.06E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
593	NC7H16+C7H15O2-3=C7H15-4+C7H15O2H-3	4.03E+12	0	17700	REV/1.44E10 0.0E0 1.5E4/
594	NC7H16+C7H15-1=C7H15-2+NC7H16	1.00E+11	0	10400	REV/1.5E11 0.0E0 1.23E4/
595	NC7H16+C7H15-1=C7H15-3+NC7H16	1.00E+11	0	10400	REV/1.5E11 0.0E0 1.23E4/
596	NC7H16+C7H15-1=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.5E11 0.0E0 1.23E4/
597	NC7H16+C7H15-2=C7H15-3+NC7H16	1.00E+11	0	10400	REV/1.0E11 0.0E0 1.04E4/
598	NC7H16+C7H15-2=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.04E4/
599	NC7H16+C7H15-3=C7H15-4+NC7H16	5.00E+10	0	10400	REV/1.0E11 0.0E0 1.04E4/
600	C7H15-1=C5H11-1+C2H4	1.23E+19	-1.91	31400	REV/1.0E11 0.0E0 8.2E3/
601	C7H15-1=C7H14-1+H	9.65E+13	-0.26	36010	REV/1.0E13 0.0E0 2.9E3/
602	C7H15-2=PC4H9+C3H6	9.76E+18	-1.79	31360	REV/1.0E11 0.0E0 8.2E3/
603	C7H15-2=C7H14-1+H	6.07E+12	0.09	36810	REV/1.0E13 0.0E0 1.2E3/
604	C7H15-2=C7H14-2+H	1.23E+13	-0.08	35640	REV/1.0E13 0.0E0 2.9E3/
605	C7H15-3=C4H8-1+NC3H7	6.17E+18	-1.71	30960	REV/1.0E11 0.0E0 7.7E3/
606	C7H15-3=C6H12-1+CH3	2.70E+17	-1.35	31480	REV/1.75E11 0.0E0 7.2E3/
607	C7H15-3=C7H14-2+H	1.23E+13	-0.08	35640	REV/1.0E13 0.0E0 2.9E3/
608	C7H15-3=C7H14-3+H	9.15E+12	-0.02	35730	REV/1.0E13 0.0E0 2.9E3/
609	C7H15-4=C2H5+C5H10-1	1.14E+18	-1.34	31430	REV/1.0E11 0.0E0 8.2E3/
610	C7H15-4=C7H14-3+H	1.82E+13	-0.02	35730	REV/1.0E13 0.0E0 2.9E3/
611	C7H15-1+O2=C7H14-1+HO2	3.00E-09	0	3000	REV/6.517E-10 1.8E-1 1.876E4/
612	C7H15-2+O2=C7H14-1+HO2	4.50E-09	0	5020	REV/1.532E-8 -1.6E-1 1.827E4/
613	C7H15-2+O2=C7H14-2+HO2	3.00E-09	0	3000	REV/5.04E-9 1.0E-2 1.912E4/
614	C7H15-3+O2=C7H14-2+HO2	3.00E-09	0	3000	REV/5.04E-9 1.0E-2 1.912E4/
615	C7H15-3+O2=C7H14-3+HO2	3.00E-09	0	3000	REV/6.769E-9 -5.0E-2 1.903E4/
616	C7H15-4+O2=C7H14-3+HO2	6.00E-09	0	3000	REV/6.795E-9 -5.0E-2 1.903E4/
617	C7H15-1=C7H15-3	1.39E+09	0.98	33760	REV/8.716E7 1.33E0 3.627E4/
618	C7H15-1=C7H15-4	2.54E+09	0.35	19760	REV/3.176E8 7.0E-1 2.227E4/
619	C7H15-2=C7H15-3	9.59E+08	1.39	39700	REV/9.587E8 1.39E0 3.97E4/
620	C7H15-1=C7H15-2	5.48E+08	1.62	38760	REV/3.445E7 1.97E0 4.127E4/
621	C7H14-1+H=C7H131-4+H2	1.30E+06	2.4	4471	REV/3.834E3 2.74E0 1.154E4/
622	C7H14-1+OH=C7H131-4+H2O	4.67E+07	1.61	-35	REV/5.963E5 1.95E0 2.219E4/
623	C7H14-1+CH3=C7H131-4+CH4	1.51E+00	3.46	5481	REV/1.163E-1 3.8E0 1.303E4/
624	C7H14-1+HO2=C7H131-4+H2O2	9.64E+03	2.6	13910	REV/7.307E2 2.62E0 4.672E3/
625	C7H14-1+CH3O2=C7H131-4+CH3O2H	9.64E+03	2.6	13910	REV/1.521E3 2.44E0 1.652E3/
626	C7H14-1+CH3O=C7H131-4+CH3OH	1.45E+11	0	4571	REV/2.062E8 3.7E-1 9.911E3/
627	C7H14-2+H=C7H132-4+H2	3.38E+05	2.36	207	REV/4.4E6 2.1E0 2.059E4/
628	C7H14-2+H=C7H132-7+H2	6.65E+05	2.54	6756	REV/3.149E4 2.53E0 1.13E4/
629	C7H14-2+OH=C7H132-4+H2O	2.76E+04	2.64	-1919	REV/1.56E6 2.38E0 3.362E4/
630	C7H14-2+OH=C7H132-7+H2O	5.27E+09	0.97	1586	REV/1.08E9 9.6E-1 2.128E4/
631	C7H14-2+CH3=C7H132-4+CH4	3.69E+00	3.31	4002	REV/1.256E3 3.05E0 2.486E4/
632	C7H14-2+CH3=C7H132-7+CH4	4.52E-01	3.65	7154	REV/5.591E-1 3.64E0 1.217E4/
633	C7H14-2+HO2=C7H132-4+H2O2	4.82E+03	2.55	10530	REV/1.615E6 1.96E0 1.46E4/

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Table B .2. (cont.)

634	C7H14-2+HO2=C7H132-7+H2O2	2.38E+04	2.55	16490	REV/2.896E4 2.21E0 4.726E3/
635	C7H14-2+CH3O2=C7H132-4+CH3O2H	4.82E+03	2.55	10530	REV/3.362E6 1.79E0 1.158E4/
636	C7H14-2+CH3O2=C7H132-7+CH3O2H	2.38E+04	2.55	16490	REV/6.03E4 2.04E0 1.706E3/
637	C7H14-2+CH3O=C7H132-4+CH3OH	4.00E+01	2.9	8609	REV/2.513E2 2.66E0 2.726E4/
638	C7H14-2+CH3O=C7H132-7+CH3OH	2.17E+11	0	6458	REV/4.953E9 2.0E-2 9.268E3/
639	C7H14-3+H=C7H132-4+H2	3.38E+05	2.36	207	REV/3.276E6 2.16E0 2.068E4/
640	C7H14-3+OH=C7H132-4+H2O	2.76E+04	2.64	-1919	REV/1.161E6 2.44E0 3.371E4/
641	C7H14-3+CH3=C7H132-4+CH4	3.69E+00	3.31	4002	REV/9.355E2 3.11E0 2.495E4/
642	C7H14-3+HO2=C7H132-4+H2O2	4.82E+03	2.55	10530	REV/1.202E6 2.03E0 1.469E4/
643	C7H14-3+CH3O2=C7H132-4+CH3O2H	4.82E+03	2.55	10530	REV/2.503E6 1.85E0 1.167E4/
644	C7H14-3+CH3O=C7H132-4+CH3OH	4.00E+01	2.9	8609	REV/1.871E2 2.73E0 2.735E4/
645	C7H131-4=C5H10-1+C2H3	2.49E+12	0.03	37300	REV/8.5E10 0.0E0 8.3E3/
646	C7H131-4=C5H81-3+C2H5	2.29E+14	-0.68	22050	REV/8.5E10 0.0E0 8.3E3/
647	C7H132-4+HO2=C7H13O2-4+OH	9.64E+12	0	0	REV/4.273E15 -1.02E0 1.543E4/
648	C7H132-4+CH3O2=C7H13O2-4+CH3O	9.64E+12	0	0	REV/4.173E17 -1.59E0 2.019E4/
649	C7H132-4+C2H5O2=C7H13O2-4+C2H5O	9.64E+12	0	0	REV/2.732E14 -6.7E-1 1.803E4/
650	C7H132-7=C2H4+C5H92-5	9.79E+17	-1.57	31160	REV/1.0E11 0.0E0 8.3E3/
651	C7H13O2-4=SC3H5CHO+NC3H7	6.32E+19	-1.93	11130	REV/1.0E11 0.0E0 9.6E3/
652	C7H13O2-4=NC3H7CHO+C3H5-S	1.01E+22	-2.46	29190	REV/1.0E11 0.0E0 9.6E3/
653	C7H14-1+OH=>CH2O+C6H13-1	1.00E+11	0	-4000	
654	C7H14-1+OH=>CH3CHO+C5H11-1	1.00E+11	0	-4000	
655	C7H14-2+OH=>CH3CHO+C5H11-1	1.00E+11	0	-4000	
656	C7H14-2+OH=>C2H5CHO+PC4H9	1.00E+11	0	-4000	
657	C7H14-3+OH=>C2H5CHO+PC4H9	1.00E+11	0	-4000	
658	C7H14-1+O=>CH2CHO+C5H11-1	1.00E+11	0	-1050	
659	C7H14-2+O=>CH3CHO+C5H10-1	1.00E+11	0	-1050	
660	C7H14-3+O=>CH3CHO+C5H10-1	1.00E+11	0	-1050	
661	C7H14-1=PC4H9+C3H5-A	3.17E+21	-1.62	75330	REV/1.0E13 0.0E0 0.0E0/
662	C7H14-2=C4H71-3+NC3H7	3.74E+21	-1.74	75710	REV/1.0E13 0.0E0 0.0E0/
663	C7H14-3=C5H91-3+C2H5	5.95E+21	-1.85	75790	REV/1.0E13 0.0E0 0.0E0/
664	C7H15O2-1=C7H15-1+O2	2.66E+20	-1.67	35400	REV/4.52E12 0.0E0 0.0E0/
665	C7H15O2-2=C7H15-2+O2	1.36E+23	-2.36	37670	REV/7.54E12 0.0E0 0.0E0/
666	C7H15O2-3=C7H15-3+O2	1.36E+23	-2.36	37670	REV/7.54E12 0.0E0 0.0E0/
667	C7H15O2-4=C7H15-4+O2	1.36E+23	-2.36	37670	REV/7.54E12 0.0E0 0.0E0/
668	C7H15-3+C7H15O2-3=2C7H15O-3	7.00E+12	0	-1000	REV/5.51E15 -7.3E-1 3.179E4/
669	C7H15-3+HO2=C7H15O-3+OH	7.00E+12	0	-1000	REV/3.081E17 -1.15E0 2.807E4/
670	C7H15-3+CH3O2=C7H15O-3+CH3O	7.00E+12	0	-1000	REV/1.927E16 -8.5E-1 3.231E4/
671	C7H15O2-1=C7H14-1+HO2	1.00E+39	-8.11	41490	
672	C7H15O2-2=C7H14-1+HO2	1.01E+43	-9.41	42490	
673	C7H15O2-2=C7H14-2+HO2	1.00E+39	-8.11	41490	
674	C7H15O2-3=C7H14-2+HO2	1.00E+39	-8.11	41490	
675	C7H15O2-3=C7H14-3+HO2	1.00E+39	-8.11	41490	
676	C7H15O2-4=C7H14-3+HO2	2.01E+39	-8.11	41490	
677	C7H15O2-1=C7H14OOH1-2	2.00E+11	0	26450	
678	C7H15O2-1=C7H14OOH1-3	2.50E+10	0	20450	
679	C7H15O2-1=C7H14OOH1-4	3.13E+09	0	18650	
680	C7H15O2-2=C7H14OOH2-1	3.00E+11	0	29000	
681	C7H15O2-2=C7H14OOH2-3	2.00E+11	0	26450	

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Table B .2. (cont.)

682	C7H15O2-2=C7H14OOH2-4	2.50E+10	0	20450	
683	C7H15O2-2=C7H14OOH2-5	3.13E+09	0	18650	
684	C7H15O2-3=C7H14OOH3-1	3.75E+10	0	24000	
685	C7H15O2-3=C7H14OOH3-2	2.00E+11	0	26450	
686	C7H15O2-3=C7H14OOH3-4	2.00E+11	0	26450	
687	C7H15O2-3=C7H14OOH3-5	2.50E+10	0	20450	
688	C7H15O2-3=C7H14OOH3-6	3.13E+09	0	18650	
689	C7H15O2-4=C7H14OOH4-1	9.38E+09	0	21950	
690	C7H15O2-4=C7H14OOH4-2	5.00E+10	0	20450	
691	C7H15O2-4=C7H14OOH4-3	4.00E+11	0	26450	
692	C7H15O2-3+HO2=C7H15O2H-3+O2	1.75E+10	0	-3275	REV/4.496E13 -8.2E-1 3.404E4/
693	H2O2+C7H15O2-3=HO2+C7H15O2H-3	2.40E+12	0	10000	REV/2.4E12 0.0E0 1.0E4/
694	C7H15O2-3+CH3O2=>C7H15O-3+CH3O+O2	1.40E+16	-1.61	1860	
695	2C7H15O2-3=>O2+2C7H15O-3	1.40E+16	-1.61	1860	
696	C7H15O2H-3=C7H15O-3+OH	1.00E+16	0	39000	REV/9.517E6 2.03E0 -6.922E3/
697	C7H15O-3=C2H5CHO+PC4H9	6.57E+17	-1.16	19370	REV/1.0E11 0.0E0 1.29E4/
698	C7H14-1+HO2=C7H14OOH1-2	2.50E+03	2.5	11200	
699	C7H14-1+HO2=C7H14OOH2-1	2.70E+03	2.5	10500	
700	C7H14-2+HO2=C7H14OOH2-3	2.70E+03	2.5	10500	
701	C7H14-2+HO2=C7H14OOH3-2	2.70E+03	2.5	10500	
702	C7H14-3+HO2=C7H14OOH3-4	2.70E+03	2.5	10500	
703	C7H14-3+HO2=C7H14OOH4-3	2.70E+03	2.5	10500	
704	C7H14OOH1-2=>C7H14O1-2+OH	6.00E+11	0	22000	
705	C7H14OOH1-3=>C7H14O1-3+OH	7.50E+10	0	15250	
706	C7H14OOH1-4=>C7H14O1-4+OH	9.38E+09	0	7000	
707	C7H14OOH2-1=>C7H14O1-2+OH	6.00E+11	0	22000	
708	C7H14OOH2-4=>C7H14O2-4+OH	7.50E+10	0	15250	
709	C7H14OOH2-5=>C7H14O2-5+OH	9.38E+09	0	7000	
710	C7H14OOH3-1=>C7H14O1-3+OH	7.50E+10	0	15250	
711	C7H14OOH3-5=>C7H14O3-5+OH	7.50E+10	0	15250	
712	C7H14OOH3-6=>C7H14O2-5+OH	9.38E+09	0	7000	
713	C7H14OOH4-1=>C7H14O1-4+OH	9.38E+09	0	7000	
714	C7H14OOH4-2=>C7H14O2-4+OH	7.50E+10	0	15250	
715	C7H14OOH1-3=>OH+CH2O+C6H12-1	2.15E+09	1.23	30370	
716	C7H14OOH2-4=>OH+CH3CHO+C5H10-1	1.55E+12	0.59	30090	
717	C7H14OOH3-1=>OH+NC4H9CHO+C2H4	8.18E+13	-0.13	31330	
718	C7H14OOH3-5=>OH+C2H5CHO+C4H8-1	2.66E+13	0.13	30430	
719	C7H14OOH4-2=>OH+NC3H7CHO+C3H6	6.19E+13	0.09	30840	
720	C7H14OOH1-3=C4H7OOH1-4+NC3H7	1.61E+12	0.54	27740	REV/2.2E3 2.48E0 6.13E3/
721	C7H14OOH1-4=>C5H10-1+C2H4+HO2	1.45E+11	0.69	30820	
722	C7H14OOH1-3O2=C7H14OOH1-3+O2	1.37E+23	-2.37	37640	REV/7.54E12 0.0E0 0.0E0/
723	C7H14OOH2-3O2=C7H14OOH2-3+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
724	C7H14OOH2-4O2=C7H14OOH2-4+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
725	C7H14OOH3-1O2=C7H14OOH3-1+O2	3.32E+20	-1.65	35280	REV/4.52E12 0.0E0 0.0E0/
726	C7H14OOH3-2O2=C7H14OOH3-2+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
727	C7H14OOH3-5O2=C7H14OOH3-5+O2	1.39E+23	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
728	C7H14OOH4-2O2=C7H14OOH4-2+O2	6.97E+22	-2.38	37600	REV/7.54E12 0.0E0 0.0E0/
729	C7H14OOH1-3O2=NC7KET13+OH	2.50E+10	0	21000	

(cont. on next page)

Table B .2. (cont.)

730	C7H14OOH2-3O2=NC7KET23+OH	1.00E+11	0	23450	
731	C7H14OOH2-4O2=NC7KET24+OH	1.25E+10	0	17450	
732	C7H14OOH3-1O2=NC7KET31+OH	1.25E+10	0	17450	
733	C7H14OOH3-2O2=NC7KET32+OH	1.00E+11	0	23450	
734	C7H14OOH3-5O2=NC7KET35+OH	1.25E+10	0	17450	
735	C7H14OOH4-2O2=NC7KET42+OH	1.25E+10	0	17450	
736	NC7KET13=>NC4H9CHO+CH2CHO+OH	1.00E+16	0	39000	
737	NC7KET23=>NC4H9CHO+CH3CO+OH	1.00E+16	0	39000	
738	NC7KET24=>NC3H7CHO+CH3COCH2+OH	1.00E+16	0	39000	
739	NC7KET31=>CH2O+NC4H9COCH2+OH	1.00E+16	0	39000	
740	NC7KET32=>CH3CHO+NC4H9CO+OH	1.00E+16	0	39000	
741	NC7KET35=>C2H5CHO+C2H5COCH2+OH	1.00E+16	0	39000	
742	NC7KET42=>CH3CHO+NC3H7COCH2+OH	1.00E+16	0	39000	
743	C7H14O1-2+OH=>PC4H9+C2H3CHO+H2O	2.50E+12	0	0	
744	C7H14O1-3+OH=>C6H12-1+HCO+H2O	2.50E+12	0	0	
745	C7H14O1-4+OH=>C5H10-1+CH2CHO+H2O	2.50E+12	0	0	
746	C7H14O2-4+OH=>CH3CO+C5H10-1+H2O	2.50E+12	0	0	
747	C7H14O2-5+OH=>CH3COCH2+C4H8-1+H2O	2.50E+12	0	0	
748	C7H14O3-5+OH=>C2H5CO+C4H8-1+H2O	2.50E+12	0	0	
749	C7H14O1-2+OH=>CH2CO+C5H11-1+H2O	2.50E+12	0	0	
750	C7H14O1-3+OH=>C2H4+NC4H9CO+H2O	2.50E+12	0	0	
751	C7H14O1-4+OH=>C2H4+NC3H7COCH2+H2O	2.50E+12	0	0	
752	C7H14O2-4+OH=>C3H6+NC3H7CO+H2O	2.50E+12	0	0	
753	C7H14O2-5+OH=>C3H6+C2H5COCH2+H2O	2.50E+12	0	0	
754	C7H14O3-5+OH=>C2H5CHO+C4H71-2+H2O	2.50E+12	0	0	
755	C7H14O1-2+HO2=>PC4H9+C2H3CHO+H2O2	5.00E+12	0	17700	
756	C7H14O1-3+HO2=>C6H12-1+HCO+H2O2	5.00E+12	0	17700	
757	C7H14O1-4+HO2=>C5H10-1+CH2CHO+H2O2	5.00E+12	0	17700	
758	C7H14O2-4+HO2=>CH3CO+C5H10-1+H2O2	5.00E+12	0	17700	
759	C7H14O2-5+HO2=>CH3COCH2+C4H8-1+H2O2	5.00E+12	0	17700	
760	C7H14O3-5+HO2=>C2H5CO+C4H8-1+H2O2	5.00E+12	0	17700	
761	C7H14O1-2+HO2=>CH2CO+C5H11-1+H2O2	5.00E+12	0	17700	
762	C7H14O1-3+HO2=>C2H4+NC4H9CO+H2O2	5.00E+12	0	17700	
763	C7H14O1-4+HO2=>C2H4+NC3H7COCH2+H2O2	5.00E+12	0	17700	
764	C7H14O2-4+HO2=>C3H6+NC3H7CO+H2O2	5.00E+12	0	17700	
765	C7H14O2-5+HO2=>C3H6+C2H5COCH2+H2O2	5.00E+12	0	17700	
766	C7H14O3-5+HO2=>C2H5CHO+C4H71-2+H2O2	5.00E+12	0	17700	
767	NC4H9COCH2=PC4H9+CH2CO	1.55E+18	-1.41	43140	REV/1.0E11 0.0E0 1.16E4/
768	C4H7OOH1-4=C4H7O1-4+OH	2.02E+20	-1.53	47040	REV/2.0E13 0.0E0 0.0E0/
769	C4H7O1-4=CH2O+C3H5-A	2.41E+16	-1.14	7550	REV/1.0E11 0.0E0 1.19E4/
770	CHCHCHO+OH=CH2CHO+HCO	1.00E+12	0	0	REV/2.719E11 2.9E-1 3.62E4/
771	O2+C6H12-1=>CH2O+NC4H9CHO	1.00E+14	0	37000	
772	C6H12-1=2C3H6	4.00E+12	0	58000	
773	C6H111-3+H=C6H12-1	1.00E+14	0	0	
774	C5H91-5+CH3=C6H12-1	1.00E+13	0	0	
775	PC4H9+C2H3=C6H12-1	1.00E+13	0	0	
776	C4H71-4+C2H5=C6H12-1	8.00E+12	0	0	
777	C6H12-1+O2=C6H111-3+HO2	2.20E+12	0	37220	

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Table B .2. (cont.)

778	C6H12-1+O2=C6H111-6+HO2	3.00E+13	0	52290	
779	C6H12-1+O=C6H111-3+OH	6.60E+05	2.43	1210	
780	C6H12-1+O=C6H111-6+OH	9.80E+05	2.43	4750	
781	C2H5+C4H6=C6H111-3	8.50E+10	0	8300	
782	C4H71-4+C2H4=C6H111-6	1.00E+11	0	8200	
783	C6H111-3+O2=C6H112O2-1	2.00E+12	0	0	
784	C6H111-3+O2=C6H111O2-3	2.00E+12	0	0	
785	C6H111-6+O2=C6H111O2-6	4.52E+12	0	0	
786	C6H12OH-1=>CH3CHO+PC4H9	1.50E+13	0	30000	
787	C6H12OH-1=>C2H5CHO+NC3H7	1.50E+13	0	30000	
789	2OH=O+H2O	3.57E+04	2.4	-2110	
790	2H+M=H2+M	1.00E+18	-1	0	Third body: AR /0.63/ Third body: C2H6 /3.0/ Third body: H2O /0.0/ Third body: CO2 /0.0/ Third body: H2 /0.0/ Third body: CH4 /2.0/
791	2H+H2=2H2	9.00E+16	-0.6	0	
792	2H+H2O=H2+H2O	6.00E+19	-1.25	0	
793	2H+CO2=H2+CO2	5.50E+20	-2	0	
794	H+OH+M=H2O+M	2.20E+22	-2	0	Third body: AR /0.38/ Third body: C2H6 /3.0/ Third body: H2O /3.65/ Third body: H2 /0.73/ Third body: CH4 /2.0/
795	H+2O2=HO2+O2	3.00E+20	-1.72	0	
796	H+O2+H2O=HO2+H2O	9.38E+18	-0.76	0	
797	H+O2+N2=HO2+N2	3.75E+20	-1.72	0	
798	H+O2+AR=HO2+AR	7.00E+17	-0.8	0	
799	HO2+H=O+H2O	3.97E+12	0	671	
800	H2O2+H=OH+H2O	1.00E+13	0	3600	
801	CO+O2=CO2+O	2.50E+12	0	47800	
802	CH+CO(+M)=HCCO(+M)	5.00E+13	0	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.69E28 -3.74E0 1.936E3/ TROE/5.757E-1 2.37E2 1.652E3 5.069E3/
803	CH+CO2=HCO+CO	3.40E+12	0	690	
804	CH2+O=HCO+H	8.00E+13	0	0	
805	CH2+OH=CH2O+H	2.00E+13	0	0	
806	CH2+HO2=CH2O+OH	2.00E+13	0	0	
807	CH2+CH=C2H2+H	4.00E+13	0	0	
808	2CH2=C2H2+H2	3.20E+13	0	0	
809	CH2(S)+N2=CH2+N2	1.50E+13	0	600	
810	CH2(S)+AR=CH2+AR	9.00E+12	0	600	
811	CH2(S)+O=CO+H2	1.50E+13	0	0	
812	CH2(S)+O=HCO+H	1.50E+13	0	0	
813	CH2(S)+O2=CO+H2O	1.20E+13	0	0	
814	CH2(S)+H2O(+M)=CH3OH(+M)	2.00E+13	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.7E38 -6.3E0 3.1E3/ TROE/1.507E-1 1.34E2 2.383E3 7.265E3/
815	CH2(S)+CO=CH2+CO	9.00E+12	0	0	

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Table B .2. (cont.)

816	CH2(S)+CO2=CH2+CO2	7.00E+12	0	0	
817	CH2(S)+CO2=CH2O+CO	1.40E+13	0	0	
818	CH2O+HO2=HCO+H2O2	1.00E+12	0	8000	
819	CH3+CH=C2H3+H	3.00E+13	0	0	
820	CH3+CH2O=CH4+HCO	3.32E+03	2.81	5860	
821	CH3+CH2=C2H4+H	4.00E+13	0	0	
822	CH3O+H(+M)=CH3OH(+M)	5.00E+13	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/8.6E28 -4.0E0 3.025E3/ TROE/8.902E-1 1.44E2 2.838E3 4.5569E4/
823	CH3O+H=CH2O+H2	2.00E+13	0	0	
824	CH3O+H=CH2(S)+H2O	1.60E+13	0	0	
825	CH3O+O=CH2O+OH	1.00E+13	0	0	
826	CH3O+OH=CH2O+H2O	5.00E+12	0	0	
827	CH3OH+H=CH3O+H2	4.20E+06	2.1	4870	
828	CH3OH+O=CH3O+OH	1.30E+05	2.5	5000	
829	CH3OH+OH=CH3O+H2O	6.30E+06	2	1500	
830	C2H+O=CH+CO	5.00E+13	0	0	
831	C2H+OH=H+HCCO	2.00E+13	0	0	
832	C2H+O2=HCO+CO	5.00E+13	0	1500	
833	C2H+H2=H+C2H2	4.90E+05	2.5	560	
834	HCCO+O2=OH+2CO	1.60E+12	0	854	
835	HCCO+CH2=C2H3+CO	3.00E+13	0	0	
836	2HCCO=C2H2+2CO	1.00E+13	0	0	
837	C2H2+O=CH2+CO	3.50E+03	2.8	500	
838	C2H3+H(+M)=C2H4(+M)	6.08E+12	0.27	280	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/1.4E30 -3.86E0 3.32E3/ TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
839	C2H3+O=CH2CO+H	3.00E+13	0	0	
840	C2H3+O2=C2H2+HO2	1.66E+14	-0.83	2540	
841	C2H3+O2=CH2CHO+O	3.50E+14	-0.611	5260	
842	C2H4+H=C2H3+H2	1.33E+06	2.53	12240	
843	C2H4+O=CH3+HCO	1.92E+07	1.83	220	
844	C2H4+OH=C2H3+H2O	3.60E+06	2	2500	
845	C2H5+O=CH3+CH2O	1.32E+14	0	0	
846	C2H5+O2=C2H4+HO2	8.40E+11	0	3875	
847	HCCO+OH=C2O+H2O	3.00E+13	0	0	
848	C2O+H=CH+CO	5.00E+13	0	0	
849	C2O+O=2CO	5.00E+13	0	0	
850	C2O+OH=2CO+H	2.00E+13	0	0	
851	C2O+O2=2CO+O	2.00E+13	0	0	
852	CH2CO+H=CH2CHO	5.40E+11	0.454	1820	
853	CH2CHO+O=CH2O+HCO	9.60E+06	1.83	220	
854	CH2CHO+O=CH2CO+OH	1.00E+13	0	0	
855	CH2CHO+OH=CH2CO+H2O	5.00E+12	0	0	

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Table B .2. (cont.)

856	CH3+HCCO=C2H4+CO	5.00E+13	0	0	
857	CH3+C2H=C3H3+H	2.41E+13	0	0	
858	CH4+C2H=C2H2+CH3	1.81E+12	0	500	
859	C2H2+CH=C3H2+H	3.00E+13	0	0	
860	C2H2+CH2=C3H3+H	1.20E+13	0	6620	
861	C2H2+CH3=C3H4-P+H	2.72E+18	-1.97	20200	
862	C2H+C2H2=H+C4H2	3.00E+14	0	0	
863	C2H2+C2H=n-C4H3	4.50E+37	-7.68	7100	
864	C2H2+C2H=i-C4H3	2.60E+44	-9.47	14650	
865	C2H2+C2H3=C4H4+H	2.00E+18	-1.68	10600	
866	C2H2+C2H3=C4H5-N	9.30E+38	-8.76	12000	
867	C2H2+C2H3=C4H5-I	1.60E+46	-10.98	18600	
868	C2H4+C2H=C4H4+H	1.20E+13	0	0	
869	C2H4+C2H3=C4H6+H	2.80E+21	-2.44	14720	
870	C2H4+O2=C2H3+HO2	4.22E+13	0	60800	
871	C2H3+H2O2=C2H4+HO2	1.21E+10	0	-596	
872	C2H3+HCO=C2H4+CO	2.50E+13	0	0	
873	2C2H3=C4H6	1.50E+42	-8.84	12483	
874	2C2H3=C4H5-N+H	2.40E+20	-2.04	15361	
875	C3H2+O=C2H2+CO	6.80E+13	0	0	
876	C3H2+CH=C4H2+H	5.00E+13	0	0	
877	C3H2+CH2=n-C4H3+H	5.00E+13	0	0	
878	C3H2+CH3=C4H4+H	5.00E+12	0	0	
879	C3H2+HCCO=n-C4H3+CO	1.00E+13	0	0	
880	C3H3+OH=C2H3+HCO	4.00E+13	0	0	
881	C3H3+HCO=C3H4-A+CO	2.50E+13	0	0	
882	C3H3+HCO=C3H4-P+CO	2.50E+13	0	0	
883	C3H3+CH=i-C4H3+H	5.00E+13	0	0	
884	C3H3+CH3(+M)=C4H612(+M)	1.50E+13	0	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.6E58 -1.194E1 9.77E3/ TROE/1.75E-1 1.3406E3 6.0E4 9.7698E3/
885	C3H4-A+H=C3H3+H2	6.63E+03	3.095	5522	
886	C3H4-A+O=CH2CO+CH2	2.00E+07	1.8	1000	
887	C3H4-A+OH=C3H3+H2O	5.30E+06	2	2000	
888	C4H+H(+M)=C4H2(+M)	1.00E+17	-1	0	Third body: AR /0.7/ Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.75E33 -4.8E0 1.9E3/ TROE/6.464E-1 1.32E2 1.315E3 5.566E3/
889	C4H+C2H2=C6H2+H	9.60E+13	0	0	
890	C4H+O=C2H+C2O	5.00E+13	0	0	
891	C4H+O2=HCCO+C2O	5.00E+13	0	1500	
892	C4H+H2=H+C4H2	4.90E+05	2.5	560	
893	C4H2+H=n-C4H3	1.10E+42	-8.72	15300	
894	H+C4H2=i-C4H3	6.30E+46	-10.15	13500	
895	C4H2+OH=H2C4O+H	6.60E+12	0	-410	

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Table B .2. (cont.)

896	C4H2+OH=C4H+H2O	3.37E+07	2	14000	
897	C4H2+CH=C5H2+H	5.00E+13	0	0	
898	C4H2+C2H=C6H2+H	9.60E+13	0	0	
899	C4H2+C2H=C6H3	4.50E+37	-7.68	7100	
900	H2C4O+H=C2H2+HCCO	5.00E+13	0	3000	
901	H2C4O+OH=CH2CO+HCCO	1.00E+07	2	2000	
902	H2C4O+O=CH2CO+C2O	2.00E+07	1.9	200	
903	n-C4H3=i-C4H3	4.10E+43	-9.49	53000	
904	n-C4H3+H=i-C4H3+H	2.50E+20	-1.67	10800	
905	n-C4H3+H=2C2H2	6.30E+25	-3.34	10014	
906	i-C4H3+H=2C2H2	2.80E+23	-2.55	10780	
907	n-C4H3+H=C4H4	2.00E+47	-10.26	13070	
908	i-C4H3+H=C4H4	3.40E+43	-9.01	12120	
909	n-C4H3+H=C4H2+H2	1.50E+13	0	0	
910	n-C4H3+OH=C4H2+H2O	2.50E+12	0	0	
911	i-C4H3+O2=HCCO+CH2CO	7.86E+16	-1.8	0	
912	n-C4H3+C2H2=l-C6H4+H	2.50E+14	-0.56	10600	
913	n-C4H3+C2H2=A1-	9.60E+70	-17.77	31300	
914	n-C4H3+C2H2=c-C6H4+H	6.90E+46	-10.01	30100	
915	C4H4+H=n-C4H3+H2	6.65E+05	2.53	12240	
916	C4H4+OH=n-C4H3+H2O	3.10E+06	2	3430	
917	C4H4+OH=i-C4H3+H2O	1.55E+06	2	430	
918	C4H4+O=C3H4-P+CO	3.00E+13	0	1808	
919	C4H4+C2H3=l-C6H6+H	2.80E+21	-2.44	14720	
920	C4H5-N=C4H5-I	1.50E+67	-16.89	59100	
921	C4H5-N+H=C4H5-I+H	3.10E+26	-3.35	17423	
922	C4H6=C4H5-I+H	5.70E+36	-6.27	112353	
923	C4H6=C4H5-N+H	5.30E+44	-8.62	123608	
924	C4H5-I+H=C4H4+H2	3.00E+13	0	0	
925	C4H5-I+OH=C4H4+H2O	5.00E+12	0	0	
926	C4H5-N+O2=>C2H4+CO+HCO	4.16E+10	0	2500	
927	C4H5-I+O2=CH2CO+CH2CHO	7.86E+16	-1.8	0	
928	C4H5-N+C2H2=l-C6H6+H	5.80E+08	1.02	10900	
929	C4H612+H=C4H6+H	2.00E+13	0	4000	
930	C4H612+H=C3H4-A+CH3	2.00E+13	0	2000	
931	C4H612+O=CH2CO+C2H4	1.20E+08	1.65	327	
932	C4H612+O=C4H5-I+OH	1.80E+11	0.7	5880	
933	C5H2+OH=>C4H2+H+CO	2.00E+13	0	0	
934	C5H2+CH=C6H2+H	5.00E+13	0	0	
935	C5H2+O2=H2C4O+CO	1.00E+12	0	0	
936	C6H2+H=C6H3	1.10E+30	-4.92	10800	
937	C6H2+O=C5H2+CO	2.70E+13	0	1720	
938	C6H2+OH=>C2H+C2H2+C2O	6.60E+12	0	-410	
939	C6H3+H=C4H2+C2H2	2.80E+23	-2.55	10780	
940	C6H3+H=l-C6H4	3.40E+43	-9.01	12120	
941	C6H3+H=C6H2+H2	3.00E+13	0	0	
942	C6H3+OH=C6H2+H2O	5.00E+12	0	0	
943	C6H3+O2=>CO+C3H2+HCCO	5.00E+11	0	0	

(cont. on next page)

Table B .2. (cont.)

944	l-C6H4+H=A1-	1.70E+78	-19.72	31400	
945	l-C6H4+H=c-C6H4+H	1.40E+54	-11.7	34500	
946	l-C6H4+H=C6H3+H2	6.65E+05	2.53	9240	
947	l-C6H4+OH=C6H3+H2O	3.10E+06	2	430	
948	c-C6H4+H=A1-	2.40E+60	-13.66	29500	
949	i-C6H5+H=C4H4+C2H2	2.80E+23	-2.55	10780	
950	i-C6H5+H=l-C6H6	3.40E+43	-9.01	12120	
951	i-C6H5+H=l-C6H4+H2	3.00E+13	0	0	
952	i-C6H5+OH=l-C6H4+H2O	5.00E+12	0	0	
953	i-C6H5+O2=>2CH2CO+C2H	7.86E+16	-1.8	0	
954	l-C6H6+H=A1+H	2.00E+18	-1.73	4500	
955	l-C6H6+H=i-C6H5+H2	3.33E+05	2.53	9240	
956	l-C6H6+OH=i-C6H5+H2O	3.10E+06	2	430	
957	A1+OH=A1-+H2O	1.60E+08	1.42	1450	
958	A1-+H(+M)=A1(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
959	n-C4H3+C4H2=A1C2H*	9.60E+70	-17.77	31300	
960	A1+C2H=A1C2H+H	5.00E+13	0	0	
961	A1-+C2H2=n-A1C2H2	7.00E+38	-8.02	16400	
962	A1-+C2H2=A1C2H+H	3.30E+33	-5.7	25500	
963	A1C2H+H=n-A1C2H2	3.00E+43	-9.22	15272	
964	A1C2H+H=i-A1C2H2	3.00E+43	-9.22	15272	
965	A1C2H+OH=A1C2H*+H2O	1.60E+08	1.42	1450	
966	A1C2H*+H(+M)=A1C2H(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
967	A1+C2H3=A1C2H3+H	7.90E+11	0	6400	
968	A1-+C2H3=A1C2H3	1.20E+27	-4.22	7235	
969	A1-+C2H3=i-A1C2H2+H	8.50E-02	4.71	18424	
970	A1-+C2H3=n-A1C2H2+H	9.40E+00	4.14	23234	
971	A1C2H3=i-A1C2H2+H	5.30E+27	-3.63	109332	
972	A1C2H3=n-A1C2H2+H	1.10E+32	-4.77	119483	
973	A1C2H3+OH=A1C2H3*+H2O	1.60E+08	1.42	1450	
974	A1C2H3*+H(+M)=A1C2H3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/6.6E75 -1.63E1 7.0E3/ TROE/1.0E0 1.0E-1 5.849E2 6.113E3/
975	A1C2H3+H=n-A1C2H2+H2	6.65E+05	2.53	12240	
976	A1C2H3+OH=n-A1C2H2+H2O	3.10E+06	2	3430	
977	n-A1C2H2+H=A1C2H+H2	1.50E+13	0	0	
978	i-A1C2H2+H=A1C2H+H2	3.00E+13	0	0	
979	n-A1C2H2+H=i-A1C2H2+H	9.90E+04	3.37	22040	
980	n-A1C2H2+OH=A1C2H+H2O	2.50E+12	0	0	

(cont. on next page)

Table B .2. (cont.)

981	i-A1C2H2+OH=A1C2H+H2O	5.00E+12	0	0	
982	A1C2H*+C2H2=A1C2H)2+H	1.80E+19	-1.67	18800	
983	A1C2H)2+H=A2-1	6.90E+63	-14.57	29900	
984	A1C2H+C2H=A1C2H)2+H	5.00E+13	0	0	
985	A1C2H3*+C2H2=A2+H	1.60E+16	-1.33	6600	
986	n-A1C2H2+C2H2=A2+H	1.60E+16	-1.33	5400	
987	A2+H=A2-2+H2	2.50E+14	0	16000	
988	A2+OH=A2-1+H2O	1.60E+08	1.42	1450	
989	A2+OH=A2-2+H2O	1.60E+08	1.42	1450	
990	A2-1+H(+M)=A2(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.8E127 -3.1434E1 1.8676E4/ TROE/2.0E-1 1.228E2 4.784E2 5.4119E3/
991	A2-2+H(+M)=A2(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/9.5E129 -3.2132E1 1.8782E4/ TROE/8.7E-1 4.927E2 1.179E2 5.652E3/
992	A2-1+H=A2-2+H	2.40E+24	-1.81	45281	
993	A2+C2H=A2C2HA+H	5.00E+13	0	0	
994	A2+C2H=A2C2HB+H	5.00E+13	0	0	
995	A2C2HB+OH=A2C2HB-J1+H2O	1.60E+08	1.42	1450	
996	A2C2HB-J1+H(+M)=A2C2HB(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/3.8E127 -3.1434E1 1.8676E4/ TROE/2.0E-1 1.228E2 4.784E2 5.4119E3/
997	A3+OH=A3-1+H2O	1.60E+08	1.42	1450	
998	A3+OH=A3-4+H2O	1.60E+08	1.42	1450	
999	A3-1+H(+M)=A3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/4.0E148 -3.7505E1 2.0551E4/ TROE/1.0E0 5.363E2 1.449E2 5.6328E3/
1000	A3-4+H(+M)=A3(+M)	1.00E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/2.1E139 -3.4803E1 1.8378E4/ TROE/1.0E-3 1.714E2 1.714E2 4.9928E3/
1001	A3-1+H=A3-4+H	3.80E+40	-6.309	61782	
1002	A4+OH=A4-4+H2O	1.60E+08	1.42	1450	
1003	A4-4+H=A4	1.00E+14	0	0	
1004	A1+A1-=P2+H	1.10E+23	-2.92	15890	
1005	A1+A1-=P2-H	3.70E+32	-6.74	9870	
1006	P2-H=P2+H	3.80E+37	-7.96	27880	
1007	2A1-=P2	2.00E+19	-2.05	2900	
1008	2A1-=P2-+H	2.30E-01	4.62	28950	
1009	P2+H=P2-+H2	2.50E+14	0	16000	

(cont. on next page)

Table B .2. (cont.)

1010	P2+OH=P2-+H2O	1.60E+08	1.42	1450	
1011	A1+O=C6H5O+H	2.20E+13	0	4530	
1012	C6H5O=CO+C5H5	2.50E+11	0	43900	
1013	C6H5O+H=CO+C5H6	3.00E+13	0	0	
1014	C6H5O+O=HCO+2C2H2+CO	3.00E+13	0	0	
1015	C6H5O+H(+M)=A1OH(+M)	2.50E+14	0	0	Third body: C2H6 /3.0/ Third body: H2O /6.0/ Third body: CO2 /2.0/ Third body: H2 /2.0/ Third body: CO /1.5/ Third body: CH4 /2.0/ LOW/1.0E94 -2.184E1 1.388E4/ TROE/4.3E-2 3.042E2 6.0E4 5.8964E3/
1016	C5H5+H(+M)=C5H6(+M)	2.60E+14	0	0	Third body: CO /1.5/ Third body: CO2 /2.0/ Third body: H2O /6.0/ Third body: H2 /2.0/ Third body: CH4 /2.0/ LOW/4.4E80 -1.828E1 1.2994E4/ TROE/6.8E-2 4.007E2 4.136E3 5.502E3/
1017	C5H5+O=C4H5-N+CO	1.00E+14	0	0	
1018	C5H5+OH=C5H4OH+H	5.00E+12	0	0	
1019	C5H5+HO2=C5H5O+OH	3.00E+13	0	0	
1020	C5H6+H=>C5H5+H2	6.00E+07	1.876	70.5	
1021	C5H5+H2=>C5H6+H	6.27E+03	2.273	23984	
1022	C5H6+O=C5H5+OH	1.80E+13	0	3080	
1023	C5H6+OH=C5H5+H2O	3.43E+09	1.18	-447	
1024	C5H5O+H=CH2O+2C2H2	3.00E+13	0	0	
1025	C5H5O+O=CO2+C4H5-N	3.00E+13	0	0	
1026	C5H4OH=C5H4O+H	2.10E+13	0	48000	
1027	C5H4OH+H=CH2O+2C2H2	3.00E+13	0	0	
1028	C5H4OH+O=CO2+C4H5-N	3.00E+13	0	0	
1029	C5H4O=CO+2C2H2	1.00E+15	0	78000	
1030	C5H4O+O=CO2+2C2H2	3.00E+13	0	0	
1031	A1C2H+OH=>A1-+CH2CO	2.18E-04	4.5	-1000	
1032	A1C2H)2+OH=>A1C2H*+CH2CO	2.18E-04	4.5	-1000	
1033	A2C2HA+OH=>A2-1+CH2CO	2.18E-04	4.5	-1000	
1034	A2C2HB+OH=>A2-2+CH2CO	2.18E-04	4.5	-1000	
1035	A1C2H+OH=>C6H5O+C2H2	1.30E+13	0	10600	
1036	A1C2H3+OH=>C6H5O+C2H4	1.30E+13	0	10600	
1037	A1C2H)2+OH=>C4H2+C6H5O	1.30E+13	0	10600	
1038	A2+OH=>A1C2H+CH2CO+H	1.30E+13	0	10600	
1039	A2C2HA+OH=>A1C2H+H2C4O+H	1.30E+13	0	10600	
1040	A2C2HB+OH=>A1C2H+H2C4O+H	1.30E+13	0	10600	
1041	A3+OH=>A2C2HB+CH2CO+H	6.50E+12	0	10600	
1042	A3+OH=>A2C2HA+CH2CO+H	6.50E+12	0	10600	
1043	A4+OH=>A3-4+CH2CO	1.30E+13	0	10600	
1044	A1C2H+O=>HCCO+A1-	2.04E+07	2	1900	
1045	A1C2H)2+O=>HCCO+A1C2H*	2.04E+07	2	1900	
1046	A1C2H3+O=>A1-+CH3+CO	1.92E+07	1.83	220	
1047	A2C2HA+O=>HCCO+A2-1	2.04E+07	2	1900	
1048	A2C2HB+O=>HCCO+A2-2	2.04E+07	2	1900	
1049	A1C2H+O=>C2H+C6H5O	2.20E+13	0	4530	
1050	A1C2H3+O=>C2H3+C6H5O	2.20E+13	0	4530	

(cont. on next page)

Table B .2. (cont.)

1051	A1C2H)2+O=>C6H5O+C4H	2.20E+13	0	4530	
1052	A2+O=>CH2CO+A1C2H	2.20E+13	0	4530	
1053	A2C2HA+O=>A1C2H)2+CH2CO	2.20E+13	0	4530	
1054	A2C2HB+O=>A1C2H)2+CH2CO	2.20E+13	0	4530	
1055	A3+O=>A2C2HA+CH2CO	1.10E+13	0	4530	
1056	A3+O=>A2C2HB+CH2CO	1.10E+13	0	4530	
1057	A4+O=>A3-4+HCCO	2.20E+13	0	4530	
1058	A1C2H*+O2=>l-C6H4+CO+HCO	2.10E+12	0	7470	
1059	A1C2H3*+O2=>l-C6H6+CO+HCO	2.10E+12	0	7470	
1060	n-A1C2H2+O2=>A1-+CO+CH2O	1.00E+11	0	0	
1061	A2-1+O2=>A1C2H+HCO+CO	2.10E+12	0	7470	
1062	A2-2+O2=>A1C2H+HCO+CO	2.10E+12	0	7470	
1063	A2C2HB-J1+O2=>A2-2+2CO	2.10E+12	0	7470	
1064	A3-4+O2=>A2C2HB+HCO+CO	2.10E+12	0	7470	
1065	A3-1+O2=>A2C2HA+HCO+CO	2.10E+12	0	7470	
1066	H2O2+OH=H2O+HO2	2.40E+00	4.042	-2162	
1067	CH3+OH=HCOH+H2	5.48E+13	0	2981	
1068	CH3+OH=CH2O+H2	2.25E+13	0	4300	
1069	CH3+H=CH2+H2	9.00E+13	0	15100	
1070	CH3+M=CH+H2+M	6.90E+14	0	82469	
1071	CH3OH(+M)=HCOH+H2(+M)	4.15E+16	-0.15	92285	Third body: H2O /16.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/4.23E44 -7.65E0 9.2911E4/ TROE/2.5E-2 1.0E-15 8.0E3 3.0E3/
1072	CH3O+O2=CH2O+HO2	6.30E+10	0	2600	
1073	HCOH+OH=HCO+H2O	2.00E+13	0	0	
1074	HCOH+H=CH2O+H	2.00E+14	0	0	
1075	HCOH+O=CO2+2H	5.00E+13	0	0	
1076	HCOH+O=CO+OH+H	3.00E+13	0	0	
1077	HCOH+O2=CO2+H+OH	5.00E+12	0	0	
1078	HCOH+O2=CO2+H2O	3.00E+13	0	0	
1079	CH2+CO2=CH2O+CO	1.10E+11	0	1000	
1080	CH2+O=CO+H2	3.00E+13	0	0	
1081	CH2+O2=CO2+2H	3.29E+21	-3.3	2868	
1082	CH2+O2=CO2+H2	1.01E+21	-3.3	1508	
1083	CH2+O2=CO+H2O	7.28E+19	-2.54	1809	
1084	CH2+O2=HCO+OH	1.29E+20	-3.3	284	
1085	2CH2=C2H2+2H	4.00E+13	0	0	
1086	CH2(S)+C2H2=C3H3+H	1.50E+14	0	0	
1087	CH2(S)+C2H4=C3H5-A+H	1.30E+14	0	0	
1088	C2H5+H=C2H4+H2	1.25E+14	0	8000	
1089	C2H5+OH=C2H4+H2O	4.00E+13	0	0	
1090	C2H5+HO2=CH3+CH2O+OH	3.00E+13	0	0	
1091	C2H3+C2H=2C2H2	3.00E+13	0	0	
1092	C2H3+CH=CH2+C2H2	5.00E+13	0	0	
1093	C2H3+CH3=C3H5-A+H	4.73E+02	3.7	5677	
1094	C2H3+CH3=C2H2+CH4	2.00E+13	0	0	
1095	2C2H3=C4H5-I+H	7.00E+13	0	0	

(cont. on next page)

Table B .2. (cont.)

1096	2C2H3=C2H4+C2H2	1.45E+13	0	0	
1097	CH2CHO+H=CH2CO+H2	4.00E+13	0	0	
1098	CH2CHO+CH3=>C2H5+CO+H	4.90E+14	-0.5	0	
1099	CH2CO+H=CH3+CO	7.00E+12	0	3011	
1100	C2H+O2=2CO+H	9.04E+12	0	-457	
1101	HCCO+H=CH2(S)+CO	1.00E+14	0	0	
1102	HCCO+O=CH+CO2	2.95E+13	0	1113	
1103	HCCO+O2=HCO+CO+O	2.50E+08	1	0	
1104	HCCO+O2=CO2+HCO	2.40E+11	0	-854	
1105	NC3H7+H=C2H5+CH3	1.00E+14	0	0	
1106	C3H6=C2H2+CH4	2.50E+12	0	70000	
1107	C3H6=C3H4-A+H2	3.00E+13	0	80000	
1108	C3H6+OH+O2=CH3CHO+CH2O+OH	3.00E+10	0	-8280	
1109	C3H6+HCO=C3H5-A+CH2O	1.08E+07	1.9	17010	
1110	CH3CHCO+OH=C2H3CO+H2O	4.00E+06	2	0	
1111	CH3CHCO+O=C2H3CO+OH	7.60E+08	1.5	8500	
1112	CH3CHCO+H=C2H3CO+H2	2.00E+05	2.5	2500	
1113	CH3CHCO+O=CH3+HCO+CO	3.00E+07	2	0	
1114	C2H3CHO+O=CH2CO+HCO+H	5.01E+07	1.76	76	
1115	C2H3CHO+H=C2H4+HCO	2.00E+13	0	3500	
1116	C2H3CO+O=C2H3+CO2	1.00E+14	0	0	
1117	C3H5-A+HO2=C2H3CHO+H+OH	1.00E+13	0	0	
1118	C3H5-A+OH=C3H4-A+H2O	1.00E+13	0	0	
1119	C3H5-A+H=C3H4-A+H2	5.00E+13	0	0	
1120	C3H5-A+O=C2H3CHO+H	1.81E+14	0	0	
1121	C3H5-A+CH3=C3H4-A+CH4	3.02E+12	-0.32	-131	
1122	C3H5-A+C2H2=C5H6+H	2.95E+32	-5.83	25733	
1123	C3H5-A+C2H3=C5H6+2H	1.59E+65	-14	61265	
1124	C3H5-T+O2=CH3CHO+HCO	1.09E+23	-3.29	3892	
1125	C3H5-T+O2=CH3CHCO+H+O	1.60E+15	-0.78	3135	
1126	C3H5-T+O=CH3CHCO+H	1.00E+14	0	0	
1127	C3H5-T+OH=C3H4-P+H2O	1.00E+13	0	0	
1128	C3H5-T+H=C3H5-A+H	1.00E+14	0	0	
1129	C3H5-S+H=C3H5-A+H	1.00E+14	0	0	
1130	C3H5-S+O2=CH3CO+CH2O	1.09E+22	-3.29	3892	
1131	C3H5-S+O=CH2CO+CH3	1.00E+14	0	0	
1132	C3H5-S+H=C3H4-P+H2	4.00E+13	0	0	
1133	C3H5-S+OH=C3H4-P+H2O	2.00E+13	0	0	
1134	C3H4-A+CH3=C3H3+CH4	1.50E+00	3.5	5600	
1135	C3H4-P+O=C2H4+CO	1.50E+13	0	2102	
1136	C3H4-A+H(+M)=C3H5-S(+M)	8.49E+12	0	2000	LOW/1.11E34 -5.0E0 4.448E3/
1137	C3H3+C2H3=C5H5+H	9.63E+40	-7.8	28820	
1138	C3H3+H(+M)=C3H4-A(+M)	1.66E+15	-0.37	0	Third body: O2 /2.0/ Third body: H2O /5.0/ Third body: C2H2 /2.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/3.36E45 -8.52E0 6.293E3/

(cont. on next page)

Table B .2. (cont.)

1139	C3H3+H(+M)=C3H4-P(+M)	1.66E+15	-0.37	0	Third body: O2 /2.0/ Third body: H2O /5.0/ Third body: C2H2 /2.0/ Third body: CO2 /3.0/ Third body: H2 /2.0/ Third body: CO /2.0/ LOW/8.78E45 -8.9E0 7.974E3/
1140	2C3H3=A1	1.30E+34	-6.5	8200	
1141	C3H3+C3H5-A=FULVENE+2H	5.56E+20	-2.535	1692	
1142	2C3H3=A1-+H	2.00E+12	0	0	
1143	CJ*CC*O=C2H2+HCO	1.00E+14	0	33000	
1144	CJ*CC*O+H=C2H3CO+H	1.00E+14	0	0	
1145	CJ*CC*O+OH=HCCCHO+H2O	1.00E+13	0	0	
1146	CJ*CC*O+H=HCCCHO+H2	2.00E+13	0	0	
1147	HCCCHO+H=C2H2+HCO	1.00E+14	0	3000	
1148	HCCCHO+OH=HCCCO+H2O	1.00E+13	0	0	
1149	HCCCHO+H=HCCCO+H2	4.00E+13	0	4200	
1150	HCCCO+O2=HCO+2CO	1.40E+09	1	0	
1151	HCCCO+H=C2H2+CO	1.00E+14	0	0	
1152	C4H8-1+O=NC3H7+HCO	1.80E+05	2.5	-1029	
1153	C4H8-1+O=C2H3CHO+CH3+H	9.67E+04	2.5	-1029	
1154	C4H8-2+O=IC3H7+HCO	2.79E+06	2.12	-1775	
1155	C4H8-2+O=CH3CO+C2H5	1.53E+07	1.87	-1476	
1156	C4H8-2+O=CH3+CH3CHCO+H	8.22E+06	1.87	-1476	
1157	C4H6+OH=C4H5-N+H2O	2.00E+07	2	5000	
1158	C4H6+OH=C4H5-I+H2O	2.00E+07	2	2000	
1159	C4H6+O=HCO+C3H5-A	6.02E+08	1.45	-858	
1160	C4H6+O=CH2CHO+C2H3	1.00E+12	0	0	
1161	C4H6+H=C4H5-N+H2	3.00E+07	2	13000	
1162	C4H6+H=C4H5-I+H2	3.00E+07	2	6000	
1163	C4H6-1+OH=CH3CHCCH+H2O	1.00E+07	2	2000	
1164	C4H6-1+H=C2H5+C2H2	1.00E+14	0	3000	
1165	C4H612+OH=C4H5-I+H2O	2.00E+07	2	1000	
1166	C4H612+OH=C4H5-2+H2O	1.00E+07	2	2000	
1167	C4H612+OH=CH3CHCCH+H2O	2.00E+07	2	2500	
1168	C4H612+H=C4H5-I+H2	5.00E+07	2	5000	
1169	C4H612+H=C4H5-2+H2	1.50E+07	2	6000	
1170	C4H612+H=CH3CHCCH+H2	3.00E+07	2	6500	
1171	CH3CHCCH+H=CH3+C3H3	1.00E+14	0	0	
1172	CH3CHCCH+O2=CH3CHCO+HCO	4.16E+10	0	2510	
1173	CH3CHCCH+OH=C4H4+H2O	3.00E+13	0	0	
1174	C4H5-I+H=CH3+C3H3	1.00E+14	0	0	
1175	C4H5-I+H=C4H5-2+H	3.00E+13	0	0	
1176	C4H5-I+C2H2=A1+H	3.00E+11	0	14900	
1177	C4H5-2+H=CH3+C3H3	1.00E+14	0	0	
1178	C4H5-2+O2=CH3CO+CH2CO	4.16E+10	0	2510	
1179	C4H5-2+H=tC4H4+H2	1.00E+14	0	8000	
1180	C4H5-2+OH=tC4H4+H2O	1.00E+13	0	0	
1181	C4H5-N+OH=C4H4+H2O	2.00E+07	2	1000	
1182	C4H5-N+H=C4H4+H2	3.00E+07	2	1000	
1183	C4H5-N+C2H2=A1+H	1.60E+16	-1.33	5400	

(cont. on next page)

Table B .2. (cont.)

1184	CH3CHCCH(+M)=C4H4+H(+M)	1.00E+13	0	49000	LOW/2.0E14 0.0E0 4.1E4/
1185	C4H5-2(+M)=tC4H4+H(+M)	1.00E+13	0	56000	LOW/2.0E14 0.0E0 4.8E4/
1186	C4H5-I(+M)=C4H4+H(+M)	1.00E+14	0	50000	LOW/2.0E15 0.0E0 4.2E4/
1187	C4H5-N(+M)=C4H4+H(+M)	1.00E+14	0	37000	LOW/1.0E14 0.0E0 3.0E4/
1188	C4H5-N+O2=CJ*CC*O+CH2O	1.00E+12	0	0	
1189	C4H5-N+O2=C4H4+HO2	1.00E+07	2	10000	
1190	C4H5-2+C3H3=C6H5CH2+H	3.00E+12	0	0	
1191	CH3CHCCH+C3H3=C6H5CH2+H	3.00E+12	0	0	
1192	2C4H5-2=CH3C6H4CH2+H	3.00E+12	0	0	
1193	2CH3CHCCH=CH3C6H4CH2+H	3.00E+12	0	0	
1194	tC4H4+OH=i-C4H3+H2O	2.00E+07	2	2000	
1195	tC4H4+H=i-C4H3+H2	3.00E+07	2	6000	
1196	C4H4+H=i-C4H3+H2	3.00E+07	2	5000	
1197	n-C4H3+O2=HCCCHO+HCO	3.00E+12	0	0	
1198	i-C4H3+OH=C4H2+H2O	3.00E+13	0	0	
1199	i-C4H3+O=CH2CO+C2H	2.00E+13	0	0	
1200	i-C4H3+O=H2C4O+H	2.00E+13	0	0	
1201	i-C4H3+H=C4H2+H2	5.00E+13	0	0	
1202	i-C4H3+CH2=C3H4-A+C2H	2.00E+13	0	0	
1203	n-C4H3(+M)=C4H2+H(+M)	1.00E+14	0	36000	LOW/1.0E14 0.0E0 3.0E4/
1204	C4H2+O=C3H2+CO	1.20E+12	0	0	
1205	C5H7=C5H6+H	3.16E+15	0	36000	
1206	C5H7=C*CCJC*C	3.16E+15	0	39500	
1207	C*CCJC*C+O=C2H3CHO+C2H3	2.00E+14	0	0	
1208	C5H6+O2=C5H5+HO2	5.00E+13	0	35400	
1209	C5H6+HO2=C5H5+H2O2	1.99E+12	0	11660	
1210	C5H6+CH3=C5H5+CH4	3.11E+11	0	5500	
1211	C5H6+C2H3=C5H5+C2H4	6.00E+12	0	0	
1212	C5H6+C4H5-N=C5H5+C4H6	6.00E+12	0	0	
1213	C5H6+C6H5O=C5H5+A1OH	3.16E+11	0	8000	
1214	C5H5+O=C5H4O+H	1.00E+14	0	0	
1215	2C5H5=>A2+2H	1.00E+12	0	6000	
1216	C5H5O=C4H5-N+CO	2.51E+11	0	43900	
1217	A1+O2=A1-+HO2	6.30E+13	0	60000	
1218	A1+H=A1-+H2	4.98E+13	0.175	10430.21	
1219	A1-+C2H4=A1C2H3+H	7.23E+01	3.5	8345	
1220	A1-+OH=C6H5O+H	5.00E+13	0	0	
1221	A1-+O=C5H5+CO	1.00E+14	0	0	
1222	A1-+O2=C6H5O+O	2.60E+13	0	6120	
1223	A1-+O2=OC6H4O+H	3.00E+13	0	8981	
1224	OC6H4O=C5H4O+CO	1.00E+15	0	78000	
1225	C6H5O+H=A1OH	1.00E+14	0	0	
1226	C6H5O+H=C24C6H6O	1.00E+14	0	0	
1227	A1OH+OH=C6H5O+H2O	2.95E+06	2	-1310	
1228	A1OH+CH3=C6H5O+CH4	1.81E+11	0	7716	
1229	A1OH+H=C6H5O+H2	1.58E+13	0	6100	
1230	A1OH+O=C6H5O+OH	2.81E+13	0	7352	
1231	A1OH+C2H3=C2H4+C6H5O	6.00E+12	0	0	

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Table B .2. (cont.)

1232	A1OH+A1-=A1+C6H5O	4.91E+12	0	4400	
1233	C24C6H6O+H=C5H7+CO	2.51E+13	0	4700	
1234	C6H5CH3=A1-+CH3	1.40E+16	0	99800	
1235	C6H5CH3+O2=C6H5CH2+HO2	2.00E+12	0	39080	
1236	C6H5CH3+OH=C6H5CH2+H2O	1.26E+13	0	2583	
1237	C6H5CH3+O=C6H5CH2+OH	5.00E+08	1.5	8000	
1238	C6H5CH3+H=C6H5CH2+H2	3.98E+02	3.44	3120	
1239	C6H5CH3+H=A1+CH3	3.50E+13	0	3690	
1240	C6H5CH3+CH3=CH4+C6H5CH2	3.16E+11	0	9500	
1241	C6H5CH3+A1-=A1+C6H5CH2	2.10E+12	0	4400	
1242	C6H5CH2+H=C6H5CH3	1.80E+14	0	0	
1243	C6H5CH2+A1OH=C6H5O+C6H5CH3	1.05E+11	0	9500	
1244	C6H5CH2+O=A1CHO+H	2.50E+14	0	0	
1245	C6H5CH2+O=A1-+CH2O	8.00E+13	0	0	
1246	C6H5CH2+HO2=A1CHO+H+OH	2.50E+14	0	0	
1247	C6H5CH2+HO2=A1-+CH2O+OH	8.00E+13	0	0	
1248	C6H5CH2+CH3=A1C2H5	1.19E+13	0	221	
1249	C6H5CH2+C3H3=C10H10	1.00E+10	0	0	
1250	C6H5CH2+A1CHO=C6H5CH3+C6H5CO	2.77E+03	2.81	5773	
1251	A1CHO+O2=C6H5CO+HO2	1.02E+13	0	38950	
1252	A1CHO+OH=C6H5CO+H2O	1.71E+09	1.18	-447	
1253	A1CHO+H=C6H5CO+H2	5.00E+13	0	4928	
1254	A1CHO+H=A1-+CH2O	2.00E+13	0	2000	
1255	A1CHO+H=A1+HCO	1.20E+13	0	5148	
1256	A1CHO+O=C6H5CO+OH	9.04E+12	0	3080	
1257	A1CHO+CH3=CH4+C6H5CO	2.77E+03	2.81	5773	
1258	A1CHO+A1-=A1+C6H5CO	7.01E+11	0	4400	
1259	C6H5CO=A1-+CO	3.98E+14	0	29400	
1260	A1C2H5+OH=A1C2H3+H2O+H	8.43E+12	0	2583	
1261	A1C2H5+H=A1C2H3+H2+H	8.00E+13	0	8235	
1262	A1C2H3+H=A1C2H3*+H2	3.03E+02	3.3	5690	
1263	A1C2H3+OH=i-A1C2H2+H2O	1.00E+07	2	2000	
1264	A1C2H3+H=i-A1C2H2+H2	2.00E+07	2	6000	
1265	A1C2H+H=A1C2H*+H2	3.03E+02	3.3	5690	
1266	A1C2H+CH3=A1C2H*+CH4	1.67E+12	0	15057	
1267	A1C2H*+C2H2=A2-1	1.07E+04	2.324	-657.3	
1268	A1C2H3*+CH3=C9H8+2H	2.00E+13	0	0	
1269	CH3C6H4CH3+OH=CH3C6H4CH2+H2O	2.95E+13	0	2623	
1270	CH3C6H4CH3+O=CH3C6H4CH2+OH	5.00E+08	1.5	8000	
1271	CH3C6H4CH3+H=CH3C6H4CH2+H2	3.98E+02	3.44	3120	
1272	CH3C6H4CH2+C2H2=C10H10+H	3.20E+11	0	7000	
1273	CH3C6H4CH2+C2H2=ch3indene+H	3.20E+11	0	7000	
1274	CH3C6H4CH2+H=CH3C6H4CH3	7.46E+13	0	78	
1275	CH3C6H4CH2+CH3=CH3C6H4C2H5	6.00E+12	0	221	
1276	C9H8+OH=C9H7+H2O	3.43E+09	1.18	-447	
1277	C9H8+O=C9H7+OH	1.81E+13	0	3080	
1278	C9H8+H=C9H7+H2	2.19E+08	1.77	3000	
1279	C9H7+O=n-A1C2H2+CO	1.00E+14	0	0	

(cont. on next page)

Table B .2. (cont.)

1280	C9H7+HO2=n-A1C2H2+CO+OH	1.00E+13	0	0	
1281	C9H7+C5H5=A3+2H	1.00E+13	0	8000	
1282	CH3C6H4C2H5+OH=CH3C6H4C2H3+H2O+H	8.43E+12	0	2583	
1283	CH3C6H4C2H5+H=CH3C6H4C2H3+H2+H	8.00E+13	0	8235	
1284	CH3C6H4C2H3+OH=C9H8+H+H2O	1.26E+13	0	2583	
1285	CH3C6H4C2H3+H=C9H8+H+H2	3.98E+02	3.44	3120	
1286	ch3indene+OH=ch3indenyl+H2O	3.43E+09	1.18	-447	
1287	ch3indene+O=ch3indenyl+OH	1.81E+13	0	3080	
1288	ch3indene+H=ch3indenyl+H2	2.19E+08	1.77	3000	
1289	ch3indene+H=C9H8+CH3	1.20E+13	0	5200	
1290	ch3indenyl+H=ch3indene	2.00E+14	0	0	
1291	ch3indenyl+C5H5=A3CH3-4+2H	1.00E+13	0	8000	
1292	C10H10+OH=C10H9+H2O	5.00E+06	2	0	
1293	C10H10+O=C10H9+OH	7.00E+11	0.7	6000	
1294	C10H10+H=C10H9+H2	2.00E+05	2.5	2500	
1295	C10H9+H=C10H10	1.00E+14	0	0	
1296	A2+H=C10H9	5.00E+14	0	5000	
1297	A2+OH=A2OH+H	9.00E+12	0	10592	
1298	A2+O=A2O+H	1.40E+13	0	1792	
1299	A2+H=A2-1+H2	4.55E+02	3.3	5690	
1300	A2-1+O2=A2O+O	1.00E+13	0	0	
1301	A2-1+OH=A2O+H	5.00E+13	0	0	
1302	A2-1+CH3=A2CH2-1+H	2.00E+13	0	0	
1303	A2-1+C2H2=A2R5+H	1.00E+20	-2.08	12000	
1304	A2-1+C2H2=A2C2HA+H	1.17E-07	5.248	-9482	
1305	A2-1+A1-=FLTN+2H	5.00E+12	0	0	
1306	A2-1+A1=FLTN+H+H2	4.00E+11	0	4000	
1307	A2O+H=A2OH	1.00E+14	0	0	
1308	A2OH+OH=A2O+H2O	2.95E+06	2	-1312	
1309	A2OH+H=A2O+H2	1.58E+13	0	6100	
1310	A2O=C9H7+CO	7.40E+11	0	43850	
1311	A2CH3-1+OH=A2CH2-1+H2O	1.27E+13	0	2583	
1312	A2CH3-1+O=A2CH2-1+OH	5.00E+08	1.5	8000	
1313	A2CH3-1+H=A2CH2-1+H2	3.98E+02	3.44	3120	
1314	A2CH3-1+H=A2+CH3	1.20E+13	0	5148	
1315	A2CH2-1+H=A2CH3-1	1.00E+14	0	0	
1316	A2CH2-1+O=A2-1+CH2O	1.00E+14	0	0	
1317	A2CH2-1+HO2=>A2-1+CH2O+OH	1.00E+13	0	0	
1318	A2CH2-1+C2H2=bz(a)ndene+H	3.20E+11	0	7000	
1319	A2CH2-1+CH3=A2C2H5	1.19E+13	0	221	
1320	A2C2H5+OH=A2C2H3+H2O+H	8.44E+12	0	2583	
1321	A2C2H5+H=A2C2H3+H2+H	8.00E+13	0	8235	
1322	A2C2H3+OH=A2CCH2+H2O	1.00E+07	2	2000	
1323	A2C2H3+H=A2CCH2+H2	2.00E+07	2	6000	
1324	A2CCH2+OH=A2C2HA+H2O	2.00E+13	0	0	
1325	A2CCH2+H=A2C2HA+H2	5.00E+13	0	0	
1326	A2C2HA+H=A2R5+H	8.46E+21	-2.614	7062.6	
1327	bz(a)ndnyl+H=bz(a)ndene	2.00E+14	0	0	

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Table B .2. (cont.)

1328	bz(a)ndene+OH=bz(a)ndnyl+H2O	3.43E+09	1.18	-447	
1329	bz(a)ndene+O=bz(a)ndnyl+OH	1.81E+13	0	3080	
1330	bz(a)ndene+H=bz(a)ndnyl+H2	2.19E+08	1.77	3000	
1331	bz(a)ndnyl+C5H5=CHRYSEN+2H	1.00E+13	0	8000	
1332	A3+OH=A3OH-1+H	9.00E+12	0	10592	
1333	A3+H=A3-1+H2	4.04E+02	3.3	5690	
1334	A3L=A3	8.00E+12	0	65000	
1335	A3-1+O2=A3O-1+O	1.00E+13	0	0	
1336	A3OH-1+OH=A3O-1+H2O	2.95E+06	2	-1310	
1337	A3OH-1+H=A3O-1+H2	1.59E+13	0	6100	
1338	A3O-1+H=A3OH-1	1.00E+14	0	0	
1339	A3O-1=bz(a)ndnyl+CO	7.40E+11	0	43850	
1340	A3-1+C2H2=A4+H	3.49E+10	0.557	5658	
1341	A3-4+CH3=hc4-p(def)pthn+2H	2.00E+13	0	0	
1342	A3CH3-4+OH=hc4-p(def)pthn+H2O+H	1.27E+13	0	2583	
1343	A3CH3-4+H=hc4-p(def)pthn+H2+H	3.98E+02	3.44	3120	
1344	A3CH3-4+H=A3+CH3	1.20E+13	0	5148	
1345	hc4-p(def)pthn+OH=hc4-p(def)pthyl+H2O	3.43E+09	1.18	-447	
1346	hc4-p(def)pthn+O=hc4-p(def)pthyl+OH	1.81E+13	0	3080	
1347	hc4-p(def)pthn+H=hc4-p(def)pthyl+H2	2.19E+08	1.77	3000	
1348	hc4-p(def)pthyl+H=hc4-p(def)pthn	2.00E+14	0	0	
1349	CHRYSEN+H=BZGFLTN+H2+H	3.03E+02	3.3	5690	
1350	CHRYSEN+OH=BZGFLTN+H2O+H	1.63E+08	1.42	1454	
1351	C5H5+CH3=>ch3cy24pd	1.50E+15	-1.527	-13500	
1352	ch3cy24pd=>C5H5+CH3	6.59E+59	-13.606	82000	
1353	ch3cy24pd+H=C5H6+CH3	1.00E+13	0	1300	
1354	FULVENE=A1	9.84E+37	-7.4	76979	
1355	FULVENE+H=A1+H	3.00E+12	0.5	2000	
1356	FULVENE+H=FULVENYL+H2	3.03E+02	3.3	5690	
1357	FULVENE+OH=FULVENYL+H2O	1.63E+08	1.42	1454	
1358	FULVENYL+H=A1-+H	1.00E+14	0	0	
1359	FULVENYL+O2=C5H4O+HCO	1.00E+12	0	0	
1360	H2+O2=2OH	1.70E+13	0	47780	
1361	O+OH+M=HO2+M	1.00E+17	0	0	
1362	H2O2+O=O2+H2O	9.55E+06	2	3970	
1363	HCO+O2=CO2+OH	3.31E+12	-0.4	0	
1364	HCO+CH3O=CH3OH+CO	9.04E+13	0	0	
1365	CH+O2=CO+OH	3.30E+13	0	0	
1366	CH2(S)+H2O=CH2+H2O	3.00E+13	0	0	
1367	CH2(S)+H=CH2+H	2.00E+14	0	0	
1368	CH2(S)+H2O2=CH3O+OH	3.01E+13	0	0	
1369	CH2(S)+HCO=CO+CH3	1.81E+13	0	0	
1370	CH2(S)+CH2O=HCO+CH3	1.20E+12	0	0	
1371	CH2(S)+O=CH+OH	3.00E+14	0	11923	
1372	CH2(S)+M=CH2+M	1.00E+13	0	0	Third body: H2O /0.0/ Third body: C2H2 /0.0/ Third body: H /0.0/
1373	CH2+CH3O=CH3+CH2O	1.81E+13	0	0	
1374	CH3+O=HCO+H2	1.26E+13	0	0	

(cont. on next page)

Table B .2. (cont.)

1375	CH3+O=CH3O	7.96E+15	-2.12	623	
1376	2CH3=C2H4+H2	1.00E+16	0	32030	
1377	CH3O+CO=CH3+CO2	1.57E+13	0	11797	
1378	CH3OH+M=CH2+H2O+M	7.00E+15	0	66444	
1379	C2H+OH=CH2+CO	1.81E+13	0	0	
1380	CH+CH2=C2H+2H	5.49E+22	-2.41	11520	
1381	HCCO+H=CH2+CO	1.00E+14	0	0	
1382	HCCO+H=HCCOH	1.81E+39	-8.039	8350	
1383	HO2+C2H=HCCO+OH	1.81E+13	0	0	
1384	C2H+O2=HCCO+O	5.00E+13	0	1500	
1385	CH2CO+O=2HCO	2.00E+13	0	2293	
1386	CH2CO+OH=CH2O+HCO	2.80E+13	0	0	
1387	CH2CO+OH=CH3O+CO	2.80E+13	0	0	
1388	C2H2+O2=C2H+HO2	1.20E+13	0	74475	
1389	CH3OH+C2H=CH3O+C2H2	1.21E+12	0	0	
1390	HO2+C2H2=CH2CO+OH	6.03E+09	0	7949	
1391	HCO+C2H=C2H2+CO	6.03E+13	0	0	
1392	CH3O+C2H=CH2O+C2H2	2.41E+13	0	0	
1393	C2H+CH2=CH+C2H2	1.81E+13	0	0	
1394	C2H3+O=C2H2+OH	3.00E+13	0	0	
1395	C2H3+O=CO+CH3	3.00E+13	0	0	
1396	CH+CH2=C2H3	3.09E+14	-1.98	620	
1397	2CH2=C2H3+H	2.00E+13	0	0	
1398	C2H3+O=HCO+CH2	3.00E+13	0	0	
1399	C2H3+CH2=CH3+C2H2	1.81E+13	0	0	
1400	2CH2=C2H4	1.11E+20	-3.43	2070	
1401	CH3O+C2H3=CH2O+C2H4	2.41E+13	0	0	
1402	CH2CO+CH2=C2H4+CO	1.60E+14	0	0	
1403	C2H3+CH2O=C2H4+HCO	5.43E+03	2.81	5862	
1404	C2H4+OH=CH3+CH2O	1.05E+12	0	-916	
1405	C2H5+O=C2H4+OH	5.00E+13	0	0	
1406	HO2+C2H5=C2H4+H2O2	3.01E+11	0	0	
1407	CH3+CH2=C2H5	1.11E+19	-3.2	1780	
1408	C2H+C2H5=C2H2+C2H4	1.81E+12	0	0	
1409	CH2+C2H5=CH3+C2H4	1.81E+13	0	0	
1410	HCO+C2H5=C2H6+CO	1.21E+14	0	0	
1411	C2H4+C2H5=C2H3+C2H6	6.32E+02	3.13	18010	
1412	CH2+C2H6=CH3+C2H5	1.20E+14	0	0	
1413	C2H6+HCO=C2H5+CH2O	4.70E+04	2.7	18233	
1414	2C2H5=C2H6+C2H4	1.39E+12	0	0	
1415	C2H3+C2H5=C2H6+C2H2	4.82E+11	0	0	
1416	C2H2+C2H5=C2H6+C2H	2.71E+11	0	23446	
1417	CH+CH2O=CH2CHO	9.64E+13	0	-517	
1418	C3H6+O=CH2CHO+CH3	1.08E+06	2.15	-795	
1419	C4H8-1+O=CH2CHO+C2H5	5.14E+06	1.95	-596	
1420	CH2CHO=CH3CO	1.00E+13	0	47100	
1421	CH3CO+O=CH3+CO2	9.64E+12	0	0	
1422	CH3CO+OH=CH2CO+H2O	1.21E+13	0	0	

(cont. on next page)

Table B .2. (cont.)

1423	CH3CO+H=CH3+HCO	3.30E+13	0	0	
1424	IC3H7+HO2=CH3CHO+CH3+OH	2.41E+13	0	0	
1425	C2H4+HO2=CH3CHO+OH	6.03E+09	0	7949	
1426	C2H3+OH=CH3CHO	3.01E+13	0	0	
1427	C3H2+O=C2H+HCO	6.80E+13	0	0	
1428	C3H2+OH=CHCHCHO	3.01E+13	0	0	
1429	C3H3=C3H2+H	5.20E+12	0	78447	
1430	C3H3+O=C3H2+OH	3.20E+12	0	0	
1431	C2H2+HCCO=C3H3+CO	1.10E+11	0	3000	
1432	C3H3+O=C2H+CH2O	7.17E+13	0	0	
1433	C3H3+O=HCCCHO+H	6.03E+13	0	0	
1434	C3H2+O=HCCCHO	6.62E+12	0	3060	
1435	CHCHCHO+H=HCCCHO+H2	1.21E+13	0	0	
1436	CHCHCHO+OH=HCCCHO+H2O	2.00E+13	0	0	
1437	C2H+CH3CO=CH3+HCCCO	1.81E+13	0	0	
1438	HCCCHO=C2H2+CO	8.51E+14	0	70940	
1439	HCCCHO+O=HCCCO+OH	5.68E+12	0	1542	
1440	C2H+CO=HCCCO	1.51E+11	0	4810	
1441	C3H3+OH=C2H3CHO	3.01E+13	0	0	
1442	C2H3CHO+H=CHCHCHO+H2	5.07E+07	1.93	12951	
1443	C2H3CHO+OH=CHCHCHO+H2O	2.02E+13	0	5955	
1444	C2H3CHO+CH3=CHCHCHO+CH4	4.16E+12	0	11128	
1445	CHCHCHO+H=C2H3CHO	5.36E+14	0	982	
1446	CHCHCHO=C2H2+HCO	2.95E+12	0	11110	
1447	NC3H7+O=C2H5CHO+H	9.64E+13	0	0	
1448	NC3H7+O2=C2H5CHO+OH	1.10E+08	0	0	
1449	C3H5-A+OH=C2H5CHO	3.01E+13	0	0	
1450	C3H4-A=C3H3+H	2.30E+12	0	69684	
1451	C3H4-P=C3H3+H	1.34E+12	0	69942	
1452	CH+C2H4=C3H4-A+H	7.17E+16	-0.84	1260	
1453	CH2+C2H2=C3H4CY	5.34E+34	-7.11	5830	
1454	CH2+C2H2=C3H4-A	1.04E+37	-7.42	6750	
1455	CH2+C2H2=C3H4-P	3.71E+37	-7.5	6850	
1456	C3H4CY=C3H4-A	1.51E+14	0	50400	
1457	C3H4CY=C3H4-P	7.08E+13	0	43700	
1458	C3H4-A+OH=HCO+C2H4	1.00E+12	0	0	
1459	C2H+CH3=C3H4-P	8.27E+46	-10	46330	
1460	C2H3+CH2=C3H4-A+H	3.00E+13	0	0	
1461	C3H4-P+C2H=C2H2+C3H3	1.00E+13	0	0	
1462	C3H4-A+O=HCO+C2H3	9.00E+12	0	1870	
1463	C3H4-P+O=CH2O+C2H2	7.50E+12	0	2102	
1464	CH+C2H4=C3H5-A	2.42E+37	-8.04	4840	
1465	C3H5-A+CH2=C4H6+H	3.01E+13	0	0	
1466	C2H+C3H5-A=C2H2+C3H4-A	1.50E-01	0	0	
1467	C2H+C3H5-A=C2H3+C3H3	2.00E+01	0	0	
1468	C2H4+CH2=C3H5-A+H	3.19E+12	0	5285.4	
1469	C3H6+CH3O=C3H5-A+CH3OH	9.00E+01	2.95	11987	
1470	C3H6+C2H=C3H4-P+C2H3	1.21E+13	0	0	

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Table B .2. (cont.)

1471	C3H6+CH2=C3H5-A+CH3	7.23E+11	0	6192	
1472	C3H6+C2H3=C3H5-A+C2H4	2.21E+00	3.5	4682	
1473	C3H5-A+HCO=C3H6+CO	6.03E+13	0	0	
1474	C3H5-A+CH3O=C3H6+CH2O	3.01E+13	0	0	
1475	C3H5-A+C2H3=C3H6+C2H2	4.82E+12	0	0	
1476	CH2+C2H5=C3H6+H	9.03E+12	0	0	
1477	CH2+C2H4=C3H6	9.03E+13	0	0	
1478	NC3H7+H=C3H6+H2	1.81E+12	0	0	
1479	NC3H7+OH=C3H6+H2O	2.41E+13	0	0	
1480	NC3H7+CH2=C3H6+CH3	1.81E+12	0	0	
1481	NC3H7+CH3=C3H6+CH4	1.14E+13	-0.32	0	
1482	NC3H7+C2H=C3H6+C2H2	6.03E+12	0	0	
1483	NC3H7+C2H3=C3H6+C2H4	1.21E+12	0	0	
1484	NC3H7+C2H5=C3H6+C2H6	1.45E+12	0	0	
1485	NC3H7+C3H5-A=2C3H6	1.45E+12	0	-131	
1486	IC3H7+H=C3H6+H2	3.61E+12	0	0	
1487	IC3H7+CH3=C3H6+CH4	9.41E+10	0.68	0	
1488	IC3H7+C2H=C3H6+C2H2	3.61E+12	0	0	
1489	IC3H7+C2H3=C3H6+C2H4	1.52E+14	-0.7	0	
1490	IC3H7+C2H5=C3H6+C2H6	2.30E+13	-0.35	0	
1491	IC3H7+C3H5-A=2C3H6	2.29E+13	-0.35	-131	
1492	IC3H7=CH3+C2H4	1.00E+12	0	34580	
1493	NC3H7+CH2=C2H4+C2H5	1.81E+13	0	0	
1494	IC3H7+C2H2=C4H6+CH3	2.77E+10	0	6504	
1495	NC3H7+C2H=C3H3+C2H5	1.21E+13	0	0	
1496	NC3H7+C2H3=C2H2+C3H8	1.21E+12	0	0	
1497	NC3H7+HCO=C3H8+CO	6.03E+13	0	0	
1498	NC3H7+CH3O=C3H8+CH2O	2.41E+13	0	0	
1499	NC3H7+CH2O=C3H8+HCO	3.01E+03	2.9	5862	
1500	NC3H7+C2H5=C3H8+C2H4	1.15E+12	0	0	
1501	2NC3H7=C3H8+C3H6	1.69E+12	0	0	
1502	NC3H7+C3H5-A=C3H4-A+C3H8	7.23E+11	0	-131	
1503	IC3H7+C2H5=C2H4+C3H8	1.84E+13	-0.35	0	
1504	IC3H7+CH2O=C3H8+HCO	1.08E+11	0	6955	
1505	IC3H7+HCO=C3H8+CO	1.21E+14	0	0	
1506	IC3H7+CH3O=C3H8+CH2O	1.21E+13	0	0	
1507	IC3H7+C2H3=C3H8+C2H2	1.52E+14	-0.7	0	
1508	IC3H7+NC3H7=C3H8+C3H6	5.13E+13	-0.35	0	
1509	2IC3H7=C3H8+C3H6	2.11E+14	-0.7	0	
1510	IC3H7+C3H5-A=C3H8+C3H4-A	4.58E+12	-0.35	-131	
1511	2C3H2=C4H2+C2H2	2.00E+13	0	85000	
1512	C4H2+C2H=C4H+C2H2	2.00E+13	0	0	
1513	C4H4+C2H=C4H2+C2H3	1.00E+13	0	0	
1514	i-C4H3+H2=C2H2+C2H3	5.01E+10	0	20000	
1515	C3H3+CH=n-C4H3+H	7.00E+13	0	0	
1516	2C2H2=C4H4	1.66E+45	-9.46	58460	
1517	2C2H3=C4H4+2H	7.83E+12	0	0	
1518	C4H4+C2H=i-C4H3+C2H2	4.00E+13	0	0	

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Table B .2. (cont.)

1519	C4H4+C2H=n-C4H3+C2H2	4.00E+13	0	0	
1520	C2H3+C2H=C4H4	9.10E+45	-9.118	21130	
1521	C4H4+C2H3=C2H4+n-C4H3	5.00E+11	0	16300	
1522	C4H4+C2H3=C2H4+i-C4H3	5.00E+11	0	16300	
1523	C4H5-I+O2=C4H4+HO2	1.20E+11	0	0	
1524	C2H3+C2H4=I-C4H7	1.32E+27	-5.58	4000	
1525	I-C4H7=C4H6+H	3.16E+13	0	34800	
1526	I-C4H7+H=C4H6+H2	1.81E+12	0	0	
1527	I-C4H7+OH=C4H6+H2O	2.41E+13	0	0	
1528	C3H6+C2H3=C4H6+CH3	7.23E+11	0	5010	
1529	C4H6+C3H3=C4H5-N+C3H4-A	1.00E+13	0	22500	
1530	C3H3+CH3=C4H6-1	5.42E+13	0	0	
1531	C3H6+C2H=C4H6-1+CH	1.21E+13	0	0	
1532	C4H6-1=C4H612	2.50E+13	0	65000	
1533	C4H6-1+O=C3H6+CO	2.00E+13	0	1659	
1534	C3H3+CH3=C4H612	3.61E+13	0	0	
1535	C4H612=C4H6	2.50E+13	0	63000	
1536	C4H612+H=C3H4-P+CH3	6.00E+12	0	2100	
1537	I-C4H7+H=C4H8-1	1.00E+14	0	0	
1538	C5H5+H=C5H4CY+H2	3.23E+07	2.095	15842	
1539	C5H5+OH=C5H4CY+H2O	2.11E+13	0	4571	
1540	C5H5+O=C5H4CY+OH	2.00E+13	0	14694	
1541	C5H5+CH3=C5H4CY+CH4	2.00E+12	0	15060	
1542	C5H4CY=C5H4L	1.00E+13	0	6000	
1543	C5H5=C3H3+C2H2	1.98E+68	-15	124887	
1544	C5H5+O=C5H5O	7.06E+04	1.03	-6960	
1545	C5H5O=C5H4O+H	2.90E+32	-6.5	21220	
1546	C5H4OH+O2=C5H4O+HO2	3.00E+13	0	5000	
1547	C5H4O+H=C4H5-N+CO	2.10E+61	-13.27	40810	
1548	C5H4O+O=C4H4+CO2	1.00E+13	0	2000	
1549	C5H6+A1-=C5H5+A1	1.00E-01	4	0	
1550	C5H6+A2-1=C5H5+A2	1.00E-01	4	0	
1551	C5H6+A2-2=C5H5+A2	1.00E-01	4	0	
1552	C5H6+C4H5-I=C5H5+C4H6	6.00E+12	0	0	
1553	C5H6+C3H5-A=C5H5+C3H6	2.00E-01	4	0	
1554	C3H5-A+C5H5=C5H6+C3H4-A	1.00E+12	0	0	
1555	C6H2+C2H=C4H+C4H2	1.00E+13	0	0	
1556	2C3H2=C6H2+H2	2.00E+13	0	85000	
1557	l-C6H4+C2H=C6H3+C2H2	2.00E+13	0	0	
1558	i-C4H3+C2H3=A1-+H	6.00E+12	0	0	
1559	A1-+HO2=C6H5O+OH	5.00E+13	0	1000	
1560	A1-+CH2O=A1+HCO	1.75E+10	0	0	
1561	A1-+H=c-C6H4+H2	9.17E-22	10.28	6175	
1562	C4H4+C2H3=A1+H	1.90E+12	0	2510	
1563	A1+C3H3=>A1-+C3H4-A	2.27E+01	3.517	24065	
1564	A1-+C3H4-A=>A1+C3H3	2.58E+00	3.73	899.32	
1565	C4H5-N+C2H3=A1+H2	1.84E-13	7.07	-3610	
1566	C4H4+C2H2=A1	4.47E+11	0	30010	

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Table B .2. (cont.)

1567	A1+O=A1-+OH	2.00E+13	0	14704	
1568	A1-+CH4=>A1+CH3	5.15E+03	2.896	15307.6	
1569	A1+CH3=>A1-+CH4	2.24E+02	3.202	6620.8	
1570	A1+OH=A1OH+H	1.56E+24	-3.19	16900	
1571	C6H5O+O=C5H5+CO2	1.00E+13	0	0	
1572	A1OH=C5H6+CO	1.00E+12	0	60802	
1573	A1OH+HO2=C6H5O+H2O2	3.00E+13	0	15000	
1574	A1OH+C4H5-N=C4H6+C6H5O	6.00E+12	0	0	
1575	A1OH+C4H5-I=C4H6+C6H5O	6.00E+12	0	0	
1576	C6H5O+O=OC6H4O+H	8.50E+13	0	0	
1577	A1-+CH3=C6H5CH2+H	3.61E+17	-0.76	20250	
1578	C4H4+C3H3=C6H5CH2	7.25E+18	-2.77	-13860	
1579	C6H5CH3+C2H3=C6H5CH2+C2H4	3.98E+12	0	8000	
1580	C4H5-N+C3H4-A=C6H5CH3+H	2.00E+11	0	3700	
1581	C4H5-N+C3H4-P=C6H5CH3+H	3.16E+11	0	3700	
1582	A1CHO=C6H5CO+H	3.98E+15	0	83660	
1583	C6H5O+CH3=C6H5OCH3	1.21E+13	0	0	
1584	A1-+CH3O=C6H5OCH3	1.21E+13	0	0	
1585	A1-+C2H=A1C2H	2.54E+17	-1.489	1541	
1586	A1-+C4H4=A1C2H+C2H3	3.20E+11	0	1350	
1587	C4H5-N+C4H2=A1C2H+H	3.16E+11	0	1800	
1588	A1C2H+OH=A1+HCCO	2.44E+03	3.02	11076	
1589	A1-+C4H4=A1C2H3+C2H	3.20E+11	0	1900	
1590	A1-+C4H6=A1C2H3+C2H3	3.20E+11	0	1900	
1591	2C4H4=A1C2H3	1.50E+14	0	38000	
1592	C4H5-N+C4H4=A1C2H3+H	3.16E+11	0	600	
1593	A1C2H3=A1+C2H2	1.58E+11	0	58440	
1594	A1-+C2H2=C8H7*2	1.10E+41	-8.61	18152	
1595	C8H7*2+H=A1C2H3	1.11E+16	-0.817	690	
1596	A1C2H3+H=C8H7*2+H2	3.23E+07	2.095	15842	
1597	A1C2H3+OH=C8H7*2+H2O	2.11E+13	0	4571	
1598	C8H7*2+O2=C6H5O+CH2CO	1.88E+12	0	7469	
1599	A1C2H3+O=A1-+CH2CHO	3.50E+13	0	2832	
1600	A1C2H3+O=n-A1C2H2+OH	7.55E+06	1.91	3736	
1601	A1C2H5+H=A1+C2H5	1.20E+13	0	5100	
1602	A1C2H5+H=A1C2H4+H2	3.97E+02	3.44	3120	
1603	A1C2H5+OH=A1C2H4+H2O	5.17E+09	1	870	
1604	A1C2H5+O2=A1C2H4+HO2	1.81E+12	0	39740	
1605	A1C2H5=A1C2H4+H	2.51E+15	0	81262	
1606	A1C2H4=A1C2H3+H	3.16E+13	0	50669	
1607	A1-+C3H3=A1C3H2+H	3.00E+12	0	0	
1608	A1C3H2+C3H3=P2-+H	3.00E+12	0	0	
1609	P2-+H=P2	2.50E+20	-1.79	2880	
1610	C8H7*2+C2H2=A2+H	4.67E+06	1.787	3262	
1611	A1-+n-C4H3=A2	6.62E+35	-6.485	15420	
1612	C6H5CH2+C3H3=A2+2H	3.00E+12	0	0	
1613	A1-+n-C4H3=A2-2+H	2.43E+31	-4.541	36700	
1614	A2+CH3=A2-1+CH4	2.00E+12	0	15060	

(cont. on next page)

Table B .2. (cont.)

1615	A2+CH3=A2-2+CH4	2.00E+12	0	15060	
1616	A2-1+O2=A2O-1+O	3.40E+30	-5.1	12950	
1617	A2-1+OH=A2O-1+H	5.00E+13	0	0	
1618	A2-2+O2=A2O-2+O	3.40E+30	-5.1	12950	
1619	A2-2+OH=A2O-2+H	5.00E+13	0	0	
1620	A2O-1+H=A2OH-1	3.47E+29	-4.303	10230	
1621	A2OH-1+H=A2O-1+H2	1.15E+14	0	12400	
1622	A2+OH=A2OH-1+H	1.56E+24	-3.19	16900	
1623	A2OH-1+OH=A2O-1+H2O	1.39E+08	1.43	-962	
1624	A2O-2+H=A2OH-2	3.47E+29	-4.303	10230	
1625	A2OH-2+H=A2O-2+H2	1.15E+14	0	12400	
1626	A2+OH=A2OH-2+H	1.56E+24	-3.19	16900	
1627	A2OH-2+OH=A2O-2+H2O	1.39E+08	1.43	-962	
1628	A2O-1=C9H7+CO	2.51E+11	0	43900	
1629	A2O-2=C9H7+CO	2.51E+11	0	43900	
1630	A2-1+CH3=A2CH3-1	1.85E+32	-5.7	8890	
1631	A2-2+C2H2=A2C2HB+H	3.89E+17	-0.87	19780	
1632	2c-C6H4=BIPHEN	4.60E+12	0	0	
1633	BIPHENH=BIPHEN+H	1.30E+16	0	33203	
1634	BIPHENH+H=BIPHEN+H2	6.02E+12	0	0	
1635	BIPHENH=A2R5+H	1.00E+13	0	20000	
1636	A2R5+H=A2R5J1+H2	3.23E+07	2.095	19800	
1637	A2R5+H=A2R5J3+H2	3.23E+07	2.095	15842	
1638	A2R5+H=A2R5J4+H2	3.23E+07	2.095	15842	
1639	A2R5+H=A2R5J5+H2	3.23E+07	2.095	15842	
1640	A2R5+OH=A2R5J1+H2O	2.10E+13	0	8600	
1641	A2R5+OH=A2R5J3+H2O	2.10E+13	0	4600	
1642	A2R5+OH=A2R5J4+H2O	2.10E+13	0	4600	
1643	A2R5+OH=A2R5J5+H2O	2.10E+13	0	4600	
1644	A2R5J1+H=A2R5	1.26E+20	-1.81	2900	
1645	A2R5J3+H=A2R5	7.00E+19	-1.73	2790	
1646	A2R5J4+H=A2R5	7.00E+19	-1.73	2790	
1647	A2R5J5+H=A2R5	7.00E+19	-1.73	2790	
1648	A2R5J1+C2H2=A2R5E1+H	1.51E+17	-0.72	20230	
1649	A2R5J3+C2H2=A2R5E3+H	1.51E+17	-0.72	20230	
1650	A2R5J4+C2H2=A2R5E4+H	1.51E+17	-0.72	20230	
1651	A2R5J5+C2H2=A2R5E5+H	4.43E-06	5.71	11070	
1652	P2-+C2H2=A3+H	1.87E+07	1.787	3262	
1653	A2C2HB+H=A2C2HB-J1+H2	3.23E+07	2.095	15842	
1654	A2C2HB-J1+C2H2=A3-1	4.67E+06	1.787	3262	
1655	A1C2H+A1-=A3+H	9.55E+11	0	4308	
1656	A1C2H*+A1=A3+H	9.55E+11	0	4308	
1657	A3+H=A3-2+H2	3.23E+07	2.095	15842	
1658	A3+H=A3-4+H2	3.23E+07	2.095	15842	
1659	A3+OH=A3-2+H2O	2.11E+13	0	4571	
1660	A3-2+H=A3	2.02E+15	-0.3	330	
1661	A2C2HB+H=A2C2HB-J3+H2	3.23E+07	2.095	15842	
1662	A2C2HB+OH=A2C2HB-J3+H2O	2.11E+13	0	4571	

(cont. on next page)

Table B .2. (cont.)

1663	A2C2HB-J3+C2H2=A3L-1	4.67E+06	1.787	3262	
1664	A2-2+C4H2=A3L-2	4.67E+06	1.787	3262	
1665	A3L+H=A3L-1+H2	3.23E+07	2.095	15842	
1666	A3L+OH=A3L-1+H2O	2.11E+13	0	4571	
1667	A3L-1+H=A3L	2.02E+15	-0.3	330	
1668	A3L+H=A3L-2+H2	3.23E+07	2.095	15842	
1669	A3L+OH=A3L-2+H2O	2.11E+13	0	4571	
1670	A3L-2+H=A3L	2.02E+15	-0.3	330	
1671	A3L+H=A3L-9+H2	3.23E+07	2.095	15842	
1672	A3L+OH=A3L-9+H2O	2.11E+13	0	4571	
1673	A3L-9+H=A3L	2.02E+15	-0.3	330	
1674	A3-1+C2H2=A3R5+H	1.83E+13	0.295	14940	
1675	A2R5E4+H=A2R5E4J5+H2	3.23E+07	2.095	15842	
1676	A2R5E4+OH=A2R5E4J5+H2O	2.10E+13	0	4600	
1677	A2R5E4J5+C2H2=A3R5J7	1.87E+07	1.787	3262	
1678	A3R5J7+H=A3R5	5.00E+13	0	0	
1679	A2R5E5+H=A2R5E5J4+H2	3.23E+07	2.095	15842	
1680	A2R5E5+OH=A2R5E5J4+H2O	2.10E+13	0	4600	
1681	A2R5E5J4+C2H2=A3R5J10	1.87E+07	1.787	3262	
1682	A3R5J10+H=A3R5	5.00E+13	0	0	
1683	A3L-1+C2H2=A3LR5+H	1.83E+13	0.295	14940	
1684	A3L-9+C2H2=A3LR5+H	1.87E+07	1.787	3262	
1685	A2R5E3+H=A2R5E3J4+H2	3.23E+07	2.095	15842	
1686	A2R5E3+OH=A2R5E3J4+H2O	2.10E+13	0	4600	
1687	A2R5E4+H=A2R5E4J3+H2	3.23E+07	2.095	15842	
1688	A2R5E4+OH=A2R5E4J3+H2O	2.10E+13	0	4600	
1689	A2R5E3J4+C2H2=A3LR5J	1.87E+07	1.787	3262	
1690	A2R5E4J3+C2H2=A3LR5J	1.87E+07	1.787	3262	
1691	A3LR5J+H=A3LR5	5.00E+13	0	0	
1692	A3-2+C2H2=A3C2H-2+H	2.08E+15	-0.13	20860	
1693	A3C2H-2+H=A3C2H-2J3+H2	3.23E+07	2.095	15842	
1694	A3C2H-2+OH=A3C2H-2J3+H2O	2.10E+13	0	4600	
1695	A3C2H-2J3+C2H2=CHRYSENJ1	1.87E+07	1.787	3262	
1696	A3-1+C2H2=A3C2H-1+H	4.63E-07	6.03	11850	
1697	A3C2H-1+H=A3C2H-1J2+H2	3.23E+07	2.095	15842	
1698	A3C2H-1+OH=A3C2H-1J2+H2O	2.10E+13	0	4600	
1699	A3C2H-1J2+C2H2=CHRYSENJ4	1.87E+07	1.787	3262	
1700	A2-2+A1C2H=CHRYSEN+H	8.51E+11	0	3986	
1701	A2+A1C2H*=CHRYSEN+H	8.51E+11	0	3986	
1702	CHRYSEN+H=CHRYSENJ1+H2	3.23E+07	2.095	15842	
1703	CHRYSEN+H=CHRYSENJ4+H2	3.23E+07	2.095	15842	
1704	CHRYSEN+H=CHRYSENJ5+H2	3.23E+07	2.095	15842	
1705	CHRYSEN+OH=CHRYSENJ1+H2O	2.10E+13	0	4600	
1706	CHRYSEN+OH=CHRYSENJ4+H2O	2.10E+13	0	4600	
1707	CHRYSEN+OH=CHRYSENJ5+H2O	2.10E+13	0	4600	
1708	CHRYSENJ1+H=CHRYSEN	5.00E+13	0	0	
1709	CHRYSENJ4+H=CHRYSEN	5.00E+13	0	0	
1710	CHRYSENJ5+H=CHRYSEN	5.00E+13	0	0	

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Table B .2. (cont.)

1711	CHRYSENJ4+C2H2=BAPYR+H	1.87E+07	1.787	3262	
1712	CHRYSENJ5+C2H2=BAPYR+H	1.87E+07	1.787	3262	
1713	A3L-1+C2H2=A3LC2H-1+H	4.63E-07	6.03	11850	
1714	A3LC2H-1+H=A3LC2H-1J2+H2	3.23E+07	2.095	15842	
1715	A3LC2H-1+OH=A3LC2H-1J2+H2O	2.10E+13	0	4600	
1716	A3LC2H-1J2+C2H2=BA3L-1	1.87E+07	1.787	3262	
1717	A3L-2+C2H2=A3LC2H-2+H	2.08E+15	-0.13	20860	
1718	A3LC2H-2+H=A3LC2H-2J1+H2	3.23E+07	2.095	15842	
1719	A3LC2H-2+OH=A3LC2H-2J1+H2O	2.10E+13	0	4600	
1720	A3LC2H-2J1+C2H2=BA3L-4	1.87E+07	1.787	3262	
1721	A2-2+A1C2H=BA3L+H	8.51E+11	0	3986	
1722	A2+A1C2H*=BA3L+H	8.51E+11	0	3986	
1723	BA3L+H=BA3L-1+H2	3.23E+07	2.095	15842	
1724	BA3L+H=BA3L-12+H2	3.23E+07	2.095	15842	
1725	BA3L+H=BA3L-4+H2	3.23E+07	2.095	15842	
1726	BA3L+OH=BA3L-1+H2O	2.10E+13	0	4600	
1727	BA3L+OH=BA3L-12+H2O	2.10E+13	0	4600	
1728	BA3L+OH=BA3L-4+H2O	2.10E+13	0	4600	
1729	BA3L-1+H=BA3L	5.00E+13	0	0	
1730	BA3L-4+H=BA3L	5.00E+13	0	0	
1731	BA3L-12+H=BA3L	5.00E+13	0	0	
1732	A3LC2H-2+H=A3LC2H-2J3+H2	3.23E+07	2.095	15842	
1733	A3LC2H-2+OH=A3LC2H-2J3+H2O	2.10E+13	0	4600	
1734	A3LC2H-2J3+C2H2=A4LJS	1.87E+07	1.787	3262	
1735	A4LJS+H=A4L	5.00E+13	0	0	
1736	A3-4+CH3=A3CH2+H	5.00E+13	0	0	
1737	A3CH2+H=A3CH3-4	1.00E+14	0	0	
1738	A3CH3-4+H=A3CH2+H2	3.98E+02	3.44	3120	
1739	A3CH3-4+OH=A3CH2+H2O	1.26E+13	0	2583	
1740	A3CH2=A3CH2R+H	1.00E+13	0	12000	
1741	A2+A1-=FLTN+H+H2	8.51E+11	0	3986	
1742	A2R5E1+H=A2R5E1J2+H2	3.23E+07	2.095	15842	
1743	A2R5E1+OH=A2R5E1J2+H2O	2.10E+13	0	4600	
1744	A2R5E1J2+C2H2=FLTNJ7	1.87E+07	1.787	3262	
1745	FLTN+H=FLTNJ1+H2	3.23E+07	2.095	15842	
1746	FLTN+OH=FLTNJ1+H2O	2.10E+13	0	4600	
1747	FLTN+H=FLTNJ3+H2	3.23E+07	2.095	15842	
1748	FLTN+OH=FLTNJ3+H2O	2.10E+13	0	4600	
1749	FLTNJ7+H=FLTN	5.00E+13	0	0	
1750	FLTNJ1+H=FLTN	5.00E+13	0	0	
1751	FLTNJ3+H=FLTN	5.00E+13	0	0	
1752	A3R5=FLTN	8.51E+12	0	62860	
1753	A3LR5=A3R5	8.51E+12	0	62860	
1754	A3LR5=FLTN	8.51E+12	0	62860	
1755	FLTNJ3+C2H2=CPCFLTN+H	1.43E+13	0.353	15790	
1756	CPCFLTN+H=CPCFLTNJS+H2	3.23E+07	2.095	15842	
1757	CPCFLTN+OH=CPCFLTNJS+H2O	2.10E+13	0	4600	
1758	CPCFLTNJS+C2H2=CPBZFLTN+H	1.87E+07	1.787	3262	

(cont. on next page)

Table B .2. (cont.)

1759	BZGFLTN-+C2H2=CPBZFLTN+H	1.43E+13	0.353	15790	
1760	CPBZFLTN+H=CPBZFLTNJS+H2	3.23E+07	2.095	15842	
1761	CPBZFLTN+OH=CPBZFLTNJS+H2O	2.10E+13	0	4600	
1762	CPBZFLTNJS+C2H2=COR1+H	1.87E+07	1.787	3262	
1763	A3-4+C2H2=A4+H	1.87E+07	1.787	3262	
1764	A1C2H*+A1C2H=A4+H	8.51E+11	0	3986	
1765	A4+OH=A4-1+H2O	1.60E+08	1.42	1450	
1766	A4+OH=A4-2+H2O	2.10E+13	0	4600	
1767	A4-2+H=A4	1.00E+14	0	0	
1768	A4-4+O2=A3-4+2CO	2.10E+12	0	7470	
1769	A4-2+C2H2=A4C2H-2+H	1.25E+17	-0.56	22560	
1770	FLTNJ1+C2H2=BZGFLTN+H	1.87E+07	1.787	3262	
1771	FLTNJ7+C2H2=BZGFLTN+H	1.87E+07	1.787	3262	
1772	BZGFLTN+H=BZGFLTN-+H2	3.23E+07	2.095	15842	
1773	BZGFLTN+OH=BZGFLTN-+H2O	2.10E+13	0	4600	
1774	A4-1+C2H2=CPCDA4+H	1.43E+13	0.353	15790	
1775	A4-4+C2H2=CPCDA4+H	1.43E+13	0.353	15790	
1776	CPCDA4+H=CPCDA4-+H2	3.23E+07	2.095	15842	
1777	CPCDA4+OH=CPCDA4-+H2O	2.10E+13	0	4600	
1778	CPCDA4-+C2H2=DCPCDA4+H	1.43E+13	0.353	15790	
1779	BZGFLTN-+C2H2=COR+H	1.87E+07	1.787	3262	
1780	CPCDA4-+C2H2=COR+H	1.43E+13	0.353	15790	
1781	COR+H=COR-+H2	3.23E+07	2.095	15842	
1782	COR+OH=COR-+H2O	2.10E+13	0	4600	
1783	COR-+C2H2=COR1+H	1.43E+13	0.353	15790	
1784	COR1+H=COR1-+H2	3.23E+07	2.095	15842	
1785	COR1+OH=COR1-+H2O	2.10E+13	0	4600	
1786	COR1-+C2H2=COR2+H	1.87E+07	1.787	3262	
1787	COR2+H=COR2-+H2	3.23E+07	2.095	15842	
1788	COR2+OH=COR2-+H2O	2.10E+13	0	4600	
1789	COR2-+C2H2=COR3+H	1.87E+07	1.787	3262	
1790	BA3L-1+C2H2=BAPYR+H	1.87E+07	1.787	3262	
1791	BA3L-12+C2H2=BAPYR+H	1.87E+07	1.787	3262	
1792	A4C2H-2+H=A4C2H-2J1+H2	3.23E+07	2.095	15842	
1793	A4C2H-2+OH=A4C2H-2J1+H2O	2.10E+13	0	4600	
1794	A4C2H-2J1+C2H2=BAPYRJS	1.87E+07	1.787	3262	
1795	BAPYRJS+H=BAPYR	5.00E+13	0	0	
1796	A2C2HA+A1C2H*=BAPYR+H	8.51E+11	0	3986	
1797	BAPYR+OH=A4C2H-2+CH2CO+H	6.50E+12	0	10600	
1798	BAPYR+O=A4C2H-2+CH2CO	1.10E+13	0	4530	
1799	BAPYRJS+O2=A4C2H-2+HCO+CO	2.10E+12	0	7470	
1800	A4C2H-2+OH=A4-2+CH2CO	2.18E-04	4.5	-1000	
1801	A4C2H-2+O=A4-2+HCCO	2.04E+07	2	1900	
1802	BAPYR+H=BAPYRJS+H2	3.23E+07	2.095	15842	
1803	BAPYR+OH=BAPYRJS+H2O	2.10E+13	0	4600	
1804	BAPYRJS+C2H2=ANTHAN+H	1.87E+07	1.787	3262	
1805	ANTHAN+OH=BAPYRJS+CH2CO	1.30E+13	0	10600	
1806	ANTHAN+O=BAPYRJS+HCCO	2.20E+13	0	4530	

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Table B .2. (cont.)

1807	C6H5CH2=FC7H6+H	4.38E+13	0.078	75900	
1808	C6H5CH2+H=FC7H6+H2	5.00E+13	0	0	
1809	FC7H6+H=>C5H5+C2H2	3.00E+14	0	0	
1810	FC7H5+H=FC7H6	2.00E+12	0	0	
1811	FC7H6+CH3=FC7H5+CH4	1.87E+04	2.724	6008	
1812	FC7H6+H=FC7H5+H2	1.90E+08	1.847	4965	
1813	FC7H5+H=C5H4CY+C2H2	1.00E+14	0	0	
1814	FC7H5(+M)=C4H2+C3H3(+M)	3.00E+12	-0.075	62300	LOW/1.0E45 8.4E0 4.75E4/
1815	A2-1+O=A2O	1.00E+14	0	0	
1816	A2-2+O=A2O	1.00E+14	0	0	
1817	A2-2+O2=A2O+O	8.90E+03	2.4	38277.512	
1818	A2-2+OH=A2O+H	3.00E+13	0	0	
1819	A2OH+O=A2O+OH	2.81E+13	0	7351.8	
1820	A2O+O=C9H6O+CO+H	1.68E+14	0	0	
1821	A2O+O2=C9H6O+CO+OH	1.08E+12	0.1	17999.5	
1822	C9H7+C3H3=A2R5+H2	4.10E+43	-9.2	15153	
1823	C9H7+HO2=C9H6O+H2O	4.76E+32	-6.5	13401	
1824	C9H7+HO2=>C9H6O+H+OH	1.31E+29	-4.7	11649.1	
1825	C9H7+O=C9H6O+H	2.80E+13	0	0	
1826	C9H7+O2=C9H6O+OH	1.38E+11	0	25320.3	
1827	C9H7+O2=>C9H6O+H+O	3.09E+15	-0.7	48740.4	
1828	C9H8+O=>C9H6O+2H	6.65E+12	-0.1	360.9	
1829	C6H5CH2+C2H2=C9H8+H	3.16E+04	2.5	11061.2	
1830	C9H8=C9H7+H	1.73E+68	-15.2	116371.9	
1831	C9H6O+H=>A1C2H3*+CO	1.79E+07	2.1	841.3	
1832	C9H8+HCO=C9H7+CH2O	1.08E+08	1.9	15999	
1833	C9H8+HO2=C9H7+H2O2	1.10E+04	2.6	12899.1	
1834	C9H8+O2=C9H7+HO2	4.00E+13	0	49639.1	
1835	FC7H6+C2H2=C9H8	1.44E+292	-78.2	245010	
1836	FC7H6+C2H2=C9H7+H	9.70E-42	16.7	37520	
1837	A1-+C3H4-A=C9H8+H	5.13E+02	3.2	2788	
1838	A1-+C3H3=C9H8	1.50E+75	-17.8	39600	
1839	A1+C3H3=C9H8+H	6.26E+09	2.61	56500	
1840	C9H8+CH3=>C9H7+CH4	2.75E+00	3.614	3380.1	
1841	C9H7+CH4=>C9H8+CH3	1.10E-02	3.883	29788	
1842	C9H8+C3H3=>C9H7+C3H4-A	5.15E-03	4.376	8021.8	
1843	C9H7+C3H4-A=>C9H8+C3H3	2.63E-03	4.563	18582	
1844	C6H5CH2=C5H5+C2H2	2.00E+14	0	70000	
1845	C5H6+H=C*CCJC*C	1.10E+14	-0.16	3100	
1846	C*CCJC*C+O2=C2H3CHO+CH2CHO	1.20E+36	-7.25	33600	
1847	C4H6-2=C4H6	3.00E+13	0	65000	
1848	C4H6-2=C4H612	3.00E+13	0	67000	
1849	C4H6-2+H=C4H612+H	2.00E+13	0	4000	
1850	C4H6-2+H=C4H5-2+H2	3.40E+05	2.5	2490	
1851	C4H6-2+H=CH3+C3H4-P	2.60E+05	2.5	1000	
1852	C4H6-2=H+C4H5-2	5.00E+15	0	87300	
1853	C4H6-2+CH3=C4H5-2+CH4	1.40E+14	0	18500	
1854	C4H5-2+C2H4=C5H6+CH3	5.00E+14	0	25000	

(cont. on next page)

Table B .2. (cont.)

1855	C4H5-2+HO2=>OH+C2H2+CH3CO	8.00E+11	0	0	
1856	A4+CH3=>A4-1+CH4	7.98E-01	3.933	11771	
1857	A4-1+CH4=>A4+CH3	4.48E-02	4.248	4277	
1858	A4+C3H3=>A4-1+C3H4-A	1.91E+01	3.529	24449.2	
1859	A4-1+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
1860	A4+H=>A4-1+H2	4.90E+08	1.884	9829.5	
1861	A4-1+H2=>A4+H	4.90E+04	2.467	2926.4	
1862	A4-1+C4H4=>BAPYR+H	1.26E+04	2.61	1649.2	
1863	A4+CH3=>A4-2+CH4	7.98E-01	3.933	11771	
1864	A4-2+CH4=>A4+CH3	4.48E-02	4.248	4277	
1865	A4+C3H3=>A4-2+C3H4-A	1.91E+01	3.529	24449.2	
1866	A4-2+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
1867	A4+H=>A4-2+H2	4.90E+08	1.884	9829.5	
1868	A4-2+H2=>A4+H	4.90E+04	2.467	2926.4	
1869	A4-2+C4H4=>BAPYR+H	1.26E+04	2.61	1649.2	
1870	A4+CH3=>A4-4+CH4	7.98E-01	3.933	11771	
1871	A4-4+CH4=>A4+CH3	4.48E-02	4.248	4277	
1872	A4+C3H3=>A4-4+C3H4-A	1.91E+01	3.529	24449.2	
1873	A4-4+C3H4-A=>A4+C3H3	1.36E+00	3.761	1088.91	
1874	A4+H=>A4-4+H2	4.90E+08	1.884	9829.5	
1875	A4-4+H2=>A4+H	4.90E+04	2.467	2926.4	
1876	C6H5CH2+C9H7=>A4+2H2	2.00E+12	0	2000	
1877	2C9H7=>A4+C2H2+H2	6.39E+29	-4.03	35205.5	
1878	A3CH2+CH2=>A4+H2+H	2.40E+14	0	0	
1879	A4-1+H=A4	1.00E+14	0	0	