Astrochemistry and combustion studies with shock waves

A dissertation submitted in partial fulfillment of the requirements

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Degree

by

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DECLARATION

I, **Deepak Kumar Singh (SR no. 02-01-02-10-11-19-1-17246)**, hereby declare that the work presented in this PhD thesis report entitled **"Astrochemistry and combustion studies with shock waves"** is the result of the work performed by me in the **Inorganic and Physical Chemistry (IPC) Department at the Indian Institute of Science, Bengaluru**, under the supervision of **Prof. E Arunan, IPC Department and Prof G. Jagadeesh, Aerospace Engineering, Department** and that it has not been submitted elsewhere for any degree or diploma. In keeping with general practice, due acknowledgments are made whenever the work is based on findings from other investigations.

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CERTIFICATE

This is to certify that the work contained in this project report entitled **"Astrochemistry and combustion studies with shock waves"** submitted by **Deepak Kumar Singh,** towards the partial requirement of **a PhD** in **Science,** has been carried out by him under my supervision at the Inorganic and Physical Chemistry Department and the Laboratory for Hypersonics and Shockwave Research lab, Aerospace Engineering Department, Indian Institute of Science, Bangalore, and no part of it has been previously submitted for a degree, diploma, or any other qualification at this university or any other institution.

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Synopsis

Shockwaves and polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the interstellar medium (ISM) and on Earth. Combustion chemistry provides the fundamental reaction routes and mechanisms for PAH formation. These fundamental chemical principles governing hydrocarbon combustion can be utilized to describe the formation and destruction of PAHs in astrophysical environments under similar shocked environments.

The primary focus of my thesis is PAHs, specifically examining the thermal processing of PAHs through shock waves in astrochemistry and the formation of aromatics, which eventually form PAHs during the pyrolysis of hydrocarbons in combustion experiments. The formation and breakdown of PAHs are assisted by shockwaves under well-defined reaction times, high temperatures, and high-pressure conditions generated via shock tube facilities. Home-built shock tube facilities in the Laboratory for Hypersonic and Shockwave Research (LHSR) lab were used to investigate high-temperature chemical kinetics and spectroscopy experiments relevant to astrochemistry and combustion. The 'single pulse nature' in the shock tube causes the reflected shock to increase the temperature up to $\sim$6000 K for $\sim$2-3 ms of dwell time. The molecules are heated behind the reflected shock wave through collisions that facilitate energy transfer between the driver gas, argon, and the sample molecule, while the wall of the shock tube remains at an ambient temperature.

Chapter 01 explores the occurrence of PAHs both on Earth and in space, highlighting the significance and justification for investigating PAHs in the pyrolysis of both hydrindane and methylcyclopentane. Chapter 02 examines the specifics of the shock tube facilities, emission spectroscopy tools, gas chro-

matography instruments, and the computational methodologies used in this thesis.

For the *astrochemistry experiments* discussed in Chapter 03, a new Material Shock Tube (MST) facility was established with an optical access chamber focusing on time-resolved and time-integrated emission spectroscopy in the UV-Vis-NIR region. The processing of interstellar dust analogues, including PAHs and fullerenes, via UV irradiation or ion/electron bombardment has been extensively studied; however, investigations through shock processing remain limited. The prototypical PAH coronene ($C_{24}H_{12}$) was selected for the shock processing study with a focus on the C_2 (Swan band) time-resolved emissions in the UV-vis region. Key findings from the research show that the shock waves enable the conversion of polycyclic aromatic PAHs into smaller hydrocarbons C_nH_x, a potential DIB carrier, and carbon clusters that subsequently recombine during the cooling phase into graphene-like structures, affecting the carbon lifecycle of the interstellar medium. The identification of C_nH_x (where n = 3–9 with a predominance of odd-numbered n, and x = 1–3) species as potential carriers of a broad green emission seen in the laboratory suggests a possible link to the 5450 Å diffuse interstellar band (DIB). The results were supported by the collection and analysis of solid residues post-shock, as well as molecular dynamics (MD) simulations conducted by various collaborators. This study establishes a foundation for future research focused on understanding the complex interactions among PAH and shocks, as well as the evolution of carbonaceous materials in the interstellar medium.

The second section of my thesis is related to combustion experiments conducted in the shock tube, as discussed in Chapters 04 and 05. For *combustion experiments*, the existing Chemical Shock Tube (CST) facility was modified

to study the thermal decomposition of hydrocarbon fuel surrogates. Trans-hydrindane (C_9H_{16}), comparable to trans-decalin ((C_9H_{18}), was selected as a bicyclic alkane substitute for diesel or jet fuel, while methyl cyclopentane ((C_6H_{12})), a branched monocyclic alkane, was chosen for naphtha or gasoline in the pyrolysis experiments. A wide variety of hydrocarbons, such as alkanes, alkenes, cycloalkanes, and aromatics, were identified through GC (gas chromatography) analysis. The experimental results were validated against a detailed kinetic model developed from high-level quantum chemistry and rate calculations, which provides fundamental insights into the elementary steps of the thermal decomposition. These studies will be further used within the laboratory to develop surrogates for ongoing RP-1 (rocket propellant) fuel experiments in the shock tube and the new flow reactor facility.

In conclusion, Chapter 06 summarizes the findings from the shock tube experiments used to develop and validate theoretical kinetic models, which in turn facilitate the interpretation of experimental observations, resulting in an in-depth understanding of PAH chemistry in both Earth and astrophysical settings. In addition to these chapters, the appendix contains the detailed reaction mechanisms for the pyrolysis of both hydrindane and methylcyclopentane.

Keywords: Astrochemistry, Combustion, PAH, Hydrocarbons, Pyrolysis, Shock waves

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Chapter 1

Introduction

1.1 Introduction and Background

This thesis examines the growth and destruction mechanisms of polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium and during combustion processes on Earth. Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous on both the Earth and in space.

PAHs in space: PAHs represent substantial components of the interstellar dust, playing a critical role in the carbon life cycle in space. In the interstellar medium (ISM), PAHs are acknowledged as a significant and widespread component. PAHs are hypothesized to originate in the outflows of evolved and dying stars and subsequently enter the ISM. PAHs are expected to account for a significant portion of the carbon present in interstellar space. PAHs are hypothesized to generate various smaller components through processes such as ultraviolet photoprocessing, shock processing, and cosmic ray destruction, including graphite, fullerenes, and a variety of smaller hydrocarbons observed in the ISM. Fullerene (C_{60}) constitutes an essential component of the dust in the interstellar medium, which has been positively identified by its spec-

tral signature and can be generated from PAHs when subjected to ultraviolet radiation.

Therefore, PAHs significantly influence the chemical composition of the dust as well as gases of the ISM and are essential to interstellar chemistry and the cosmic life cycle. They function as diagnostic tracers of the surrounding conditions in astrophysical environments, providing insights from various infrared emission studies in the interstellar medium. Their unique spectral signatures, particularly in the infrared spectrum, aid in identifying the conditions present in different regions of the interstellar medium.

PAHs on Earth: Polycyclic aromatic hydrocarbons (PAHs) are the most prevalent chemical compounds naturally occurring in crude oil, coal deposits, and other readily available carbonaceous materials on Earth. PAHs from man-made sources are primarily derived through combustion processes. At elevated temperatures, fuel molecules decompose, leading to the formation of smaller hydrocarbon fragments. Smaller hydrocarbon fragments recombine and undergo cyclization, resulting in the formation of aromatic rings such as benzene and toluene. Aromatic rings interact through various mechanisms to form PAHs.

PAHs act as intermediates in the pyrolysis and oxidation of fuel molecules, serving as precursors to soot particles. Soot formation involves the development of PAHs into larger structures, subsequently leading to their aggregation into solid particles. PAHs are recognized as carcinogenic agents, capable of inducing cancer. A substantial category of chemicals exists, many of which exhibit genotoxic, mutagenic, and teratogenic properties, in addition to their carcinogenic potential. PAHs can further induce cancer through their interaction with DNA, resulting in alterations that may trigger tumor development

[5].

What is a PAH?

PAHs are hydrocarbons characterized by carbon atoms organized in a honeycomb lattice structure formed by fused six-membered aromatic rings, with hydrogen atoms located at the edges.

The two primary categories of PAHs are depicted in Figure 1.1. The compact structure of pericondensed PAHs (left side) is characterized by C-atoms forming either two or three distinct rings. Coronene, coroannulene, and circumcoronene are constituents of this category of PAHs. Their structure facilitates complete electron delocalization and robust aromatic bonding among adjacent carbon atoms, making them very stable. Their core structure is cyclic and surrounded by many rings. The absence of a C-atom in more than two rings differentiates the open structures of catacondensed PAHs (right side). The aromatic rings are arranged in either linear chains (such as naphthalene, anthracene, tetracene, etc.) or bending rows (such as phenanthrene, tetraphene, etc.) [6, 7, 1] The investigation of PAH formation and degradation is essential for understanding processes occurring on Earth and within the interstellar medium. Similar mechanisms exist in both environments under similar shock conditions; thus, the study is analogous. Part 01 (Astrochemistry (Section 1.2)) of the study addresses the problem within the astrophysical environment, and Part 02 (Combustion (Section 1.3)) investigates the phenomenon in combustion settings.

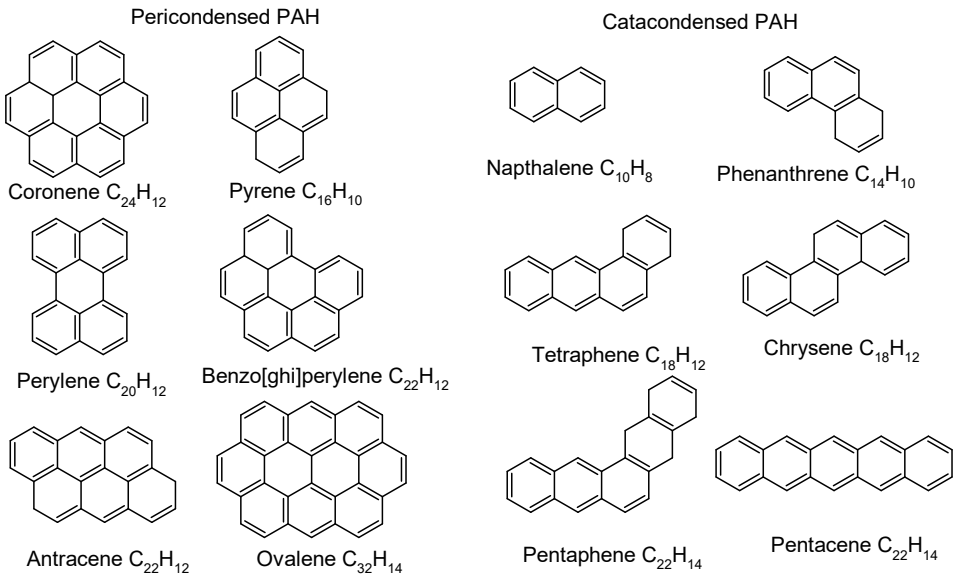


Figure 1.1: PAH structures: Pericondensed and catacondensed PAHs. Figure reproduced from [1], with permission

1.2 Astrochemistry

This section of the chapter examines the PAH in the ISM. ISM consists of the matter and radiation that exist in the space between star systems within a galaxy. The ISM is primarily composed of gas, accounting for around 99% of its mass, with dust making up the remaining 1%. In the interstellar medium, 91% of atoms are hydrogen, 8.9% are helium, and 0.1% consist of heavier elements, referred to as "metals" in astronomical terminology. By mass, the gas mostly consists of hydrogen (about 70%) and helium (around 28%), with trace amounts of heavier elements (about 1%). H has an atomic mass of approximately 1, while He has an atomic mass of about 4. A single He atom possesses approximately four times the mass of an H atom. Although H atoms are abundant, the greater mass of the He atom leads to a more substantial impact on the total mass of the interstellar medium than on the total atomic count. [8].

PAHs represent substantial components of the 1% interstellar dust, playing

a critical role in the carbon life cycle in space. PAHs are hypothesized to originate in the outflows of evolved and dying stars and subsequently enter the ISM. Fullerenes are hypothesized to form from PAHs upon exposure to ultraviolet radiation, indicating a relationship between PAHs and fullerenes in the interstellar medium through a top-down formation mechanism. PAHs are acknowledged as a significant and widespread component, whereas fullerenes, especially C_{60}, exist in smaller quantities. The coexistence of PAHs and fullerenes is well established through observations in ISM; however, the transition from PAHs to fullerenes in space remains inadequately understood [8]. Therefore, in conjunction with the discussion of PAH, we will also integrate studies related to fullerene to understand the evolution of PAH in ISM through laboratory studies.

Before discussing the observations and processing methods of PAH in the ISM, all processes can be broadly categorized into three distinct categories. Subsequent to energy exchange via UV photons, ions, or shocks, etc., an energetically excited molecule may experience additional cooling and participate in various reactions, including statistical fragmentation (timescale of picoseconds (ps) (for eg., UV photodissociation reactions)), non-statistical fragmentation (occurring on femtosecond (fs) timescales)(for eg. knockout driven reactions)), or photon emission (such as IR emissions with much longer time scales).

PAH excitation mechanisms and IR spectrum:

Prior to examining the observations in this section, it is essential to address the photophysics that occur following UV photon absorption.

Consider a neutral PAH molecule in its singlet electronic ground state, S_0. UV radiation absorption in the ISM at energies corresponding to the molecule's specific electronic energy levels allows the transitions to higher electronic states, such as S_1, S_2, or thereafter. The PAH molecule is currently in an excited state

and can undergo numerous de-excitation processes, including ionization and photodissociation, with the predominant pathway determined by its immediate surroundings. For example, on Earth, collisional de-excitation is typically the predominant process. In the ISM's collision-free environment of space, the primary focus in this section will be placed on infrared fluorescence.

Internal conversion (IC) from the excited electronic state results in a vibrationally excited molecule in a lower-lying electronic state (S_0). Fluorescence may also subsequently occur in singlet states (S_1 to S_0). Both fluorescence and internal conversion processes are the competing relaxation pathways from the first excited singlet state (S_1) back to the ground singlet state (S_0). Fluorescence is a radiative process, while internal conversion is a non-radiative process. The molecule is also capable of undergoing intersystem crossing (ISC) to an excited vibrational state of an electronic state characterized by a different multiplicity, which is the triplet system (T_1). If intersystem crossing has occurred, the molecule remains electronically excited. The final radiative decay step is characterized by phosphorescence, involving the emission of photons. All the processes will ultimately result in radiative or non-radiative relaxation to the ground vibrational state of the corresponding electronic state through a series of vibrational level transitions.

1.2.1 Observations

Observation for PAH

Infrared radiation is considered one of several potential mechanisms in the energetic interactions of molecules within the ISM. The excited molecule will move to a lower-lying electronic state through internal conversion, leaving most of the initial excitation energy in the form of vibrational energy. Fol-

lowing photoexcitation by UV radiation, electronic relaxation primarily occurs through nonradiative mechanisms. In this process, the electronic energy is converted to vibrational energy, which is randomly distributed across all vibrational degrees of freedom within the electronic ground state. Following that, the molecule that is highly vibrationally excited undergoes a cooling process, primarily through infrared emission in specific vibrational modes, such as C-H and C-C stretching, among others. Comprehensive analyses of these features are presented, along with appropriate examples.

The infrared spectrum of various objects and regions that absorb ultraviolet radiation displays broad emission features at 3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 μm, along with several weaker features, as illustrated in Figure 1.2. For nearly a decade, the carriers of these features were mysterious and led to their collective classification as Unidentified InfraRed bands (UIR). The combination of astronomical spectra with laboratory spectroscopy and quantum chemistry computations of transitions facilitated the identification of polycyclic aromatic hydrocarbons (PAHs) as the carriers of the observed UIR bands. The found characteristics indicated the stretching and bending vibrational modes related to aromatic hydrocarbon substances [10, 7].

Several details are provided here: The 3 μm sections are characteristic of C-H stretching modes: the 3.3 μm band correlates to the C-H stretching mode in aromatic compounds, while the 3.4 μm band may arise from aliphatic groups acting as substituents on the PAHs or from PAHs with additional hydrogen atoms bonded to specific carbons. The region of 6.1–6.5 μm is defined by pure C-C stretching modes, whereas the extended range of 6.5–8.5 μm encompasses mixed vibrations, including C-C stretching and C-H in-plane bending modes, with C-H in-plane wagging modes producing bands in

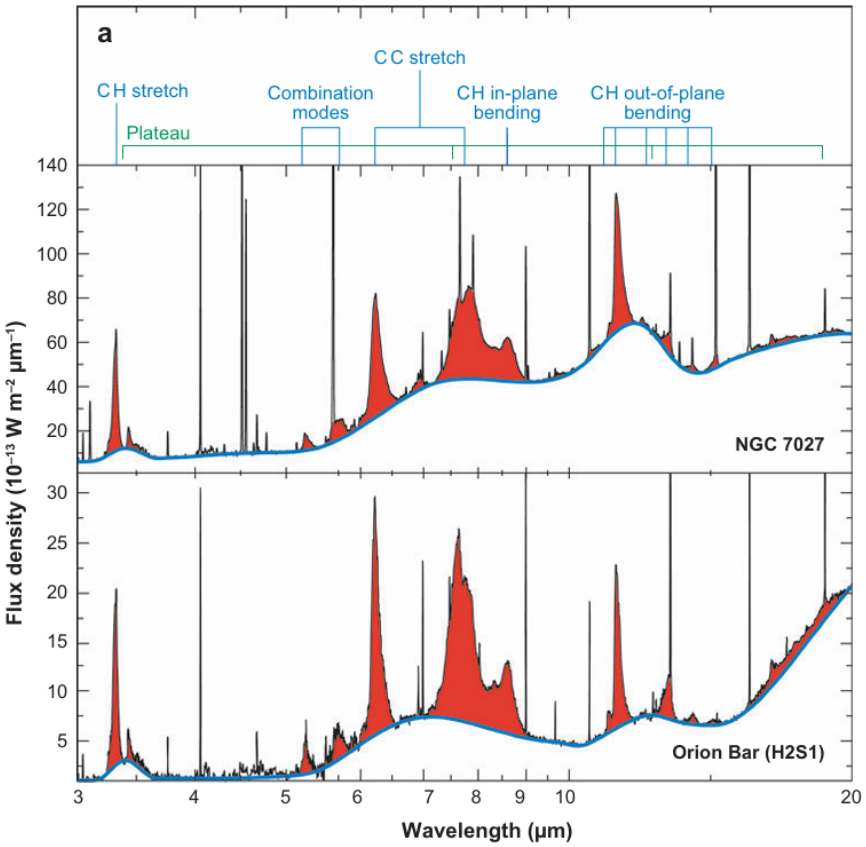


Figure 1.2: The mid-infrared spectra of the photodissociation region in the Orion Bar and in the planetary nebulae NGC 7027. The spectra are dominated by a rich set of emission features, (almost) universally attributed to vibrational modes of polycyclic aromatic hydrocarbon molecules (top panel). The narrow features are atomic or ionic lines originating in the HII region or photodissociation region. Figure reproduced from [6], adapted from [9] with permission

the 8.3–8.9 μm range. Beyond roughly 11–13 μm, emission bands correspond to in-plane and out-of-plane bending motions of the carbon structure; hence, these modes demonstrate enhanced molecular selectivity, particularly at longer wavelengths. A detailed overview of the vibrational modes of PAH, including the experimental methods and theoretical methods utilized in their study, can be found in the review [6].

More recently, the discovery through radio observations in the cold and dense interstellar cloud TMC-1 of two isomers of cyanonapthalene [$C_{10}H_7CN$, 11], of indene [C_9H_8, 12, 13], of isomers of cyano-acenaphtylene [$C_{12}H_8$, 14], of isomers of cyano-pyrene [$C_{16}H_9CN$, 15, 16], and of cyano-coronene [$C_{24}H_{11}CN$, 17] has brought decisive proof of the presence of PAHs in the interstellar medium (ISM).

Such astronomical observations suggest that PAHs are abundant and widespread in photodissociation regions associated with massive star-forming regions, planetary nebulae, and protoplanetary disks [18, 19, 20, 9, 21, 22, 23]. Photodissociation regions (PDRs) have been investigated with regard to the regions where the impact of stellar far-ultraviolet (FUV) ($6\,\mathrm{eV}<h\nu<13.6\,\mathrm{eV}$) photons affects the structure, chemistry, thermal equilibrium, and evolution of the neutral interstellar medium in galaxies. FUV photons illumine star-forming regions, producing infrared emissions that signify the environment and may substantially affect the evolution of the star formation process involving PAHs and other substances [6]. The dominant viewpoint is that large PAHs cause this IR emission. Photostability studies suggest a lower limit of about 50 carbon atoms [e.g., 24], whereas a more recent spectral study indicated sizes in the range of 40–55 carbon atoms [25]. A large fraction of carbon, up to 10%, might be locked up in these species [6].

Observations for fullerene

Fullerene is a carbon allotrope accidentally identified through the laser ablation of graphite, with the objective of understanding the synthesis mechanisms of long-chain carbon molecules in the interstellar medium or circumstellar shells [26]. The clear identification of all four infrared active modes of C_{60} at 7.0, 8.5, 17.4, and 18.9 μm was accomplished by analyzing Spitzer IRS spectra of the planetary nebula Tc1 ([27]). Similar spectral features have been identified in reflection nebulae and young stellar object circumstellar environments [28, 29, 30], the diffuse interstellar medium [31], and young stellar objects and Herbig Ae/Be stars [30]. The IR features associated with fullerene cations, C_{60}^+, at 6.4, 7.1, 8.2, and 10.5 μm were previously recorded [32, 33].

The omnipresence of PAHs along with some fullerenes in space has also led to considering them as potential carriers of diffuse interstellar bands (DIBs) [see e.g. 34]. Diffuse interstellar bands are ubiquitous absorption features seen in lines of sight crossing diffuse interstellar clouds and spanning the near ultraviolet to near infrared range [35, 36, 37, 25, 38, 39]. Despite many attempts to link DIBs to PAHs and fullerene, no decisive matches with cold gas-phase laboratory spectral signatures have been found [e.g. 40, 41, 42, 43, 44]. As of today, only four DIBs have been assigned, all to C_{60}^+. They include the λ9577 and λ9632 strong DIBs [45, 46, 47, 33]. Among the other candidates, carbon chains appear promising ones [48, 49], although past tentative assignments to DIBs have also been inconclusive [see e.g. 4].

While considerable effort has been devoted to measuring the spectral signature of PAHs or derivatives, many studies have sought to explore their physical-chemistry properties. Beyond their formation pathways, which still elude us, many gaps persist in our understanding on how PAHs evolve and are altered.

UV irradiation, cosmic ray bombardment, and shocks count among the key drivers of PAH destruction.

1.2.2 Formation processes

PAH formation

The exact mechanisms that lead to the generation of these large cyclic species in space remain, however, debated and have stimulated decades of laboratory work. Outflows of carbon-rich stars provide physical and chemical settings close to combustion and flame environments, favorable to the formation of PAHs through a bottom-up process. Small carbon-containing molecules and radicals, which are abundant in these outflows, can undergo a series of reactions to form ringed structures, which can then grow into PAHs [50, 51]. Among the key processes, hydrogen-abstraction/acetylene-addition (HACA) is considered to be a crucial route for forming PAHs [52].

A large fraction of PAHs is additionally directly produced at low temperature in interstellar cold clouds, as suggested by the latest isotopic measurements of the Ryugu samples [53]. Recent observations mainly carried out with the Yebes 40-m radiotelescope indicate that aromatics are widespread in cold clouds [54], independently supporting this finding.

Laboratory experiments combined with computation methods have also led to the proposition of alternative top-down scenarios for PAH production in circumstellar envelopes. These hot environments could for instance promote the formation of hydrogenated aromatic carbon nanograins and inject them in the ISM [55]. They could then later on release carbon chains and PAHs when reaching photon dominated regions. PAHs could be produced too from

graphene etching onto SiC grains in the hot inner shells of evolved stars [56]. Radiation pressure from the star could then drive the grains to the exterior of the envelope, where they could be further processed by external UV photons and H atoms, liberating PAHs in the gas-phase.

Fullerene formation

Fullerenes are expected to form in high-temperature, hydrogen-deficient, and carbon-abundant environments, such as Wolf-Rayet stars [57, 58] or R Coronae stars [59]. Garcia et al. [29] demonstrated that fullerenes may be generated in hydrogen-rich planetary nebulae, whereas Berne et al. [60] proposed that C_{60} fullerenes may originate in the cold conditions of the interstellar medium (ISM) and that large polycyclic aromatic hydrocarbons can be converted into graphene and subsequently into fullerenes as a result of ultraviolet radiation.

In the laboratory, there are several methods to generate fullerenes. Kratschmer et al. [61] demonstrated that fullerenes can be efficiently synthesized through the arc vaporization of graphite. This method is capable of producing substantial amounts of carbon soot that contains fullerenes. Fullerenes can also be formed by the condensation of a plume produced by laser ablation of a graphite target [26, 58], or by condensation of products of laser-induced pyrolysis of hydrocarbons [58]. In such experiments, two temperature regimes are identified. Below 1700 K, condensation by-products are mainly polycyclic aromatic hydrocarbons (PAHs). Above 3500 K, fullerene-like carbon grains and fullerene compounds are formed. Micelotta et al. [62] suggested that fullerenes may be produced in the ISM from hydrogenated amorphous carbon (a-C:H). The experimental study of electron bombardment of graphene in turn induces the curving of the graphene into a bowl-shaped structure [63].

Some other routes could also be considered. The theoretical study of [64] suggests that the vibrational excitation of PAHs by impacting ions or electrons may lead to restructuring into more stable fullerene-type species. Further theoretical investigations of PAHs in a hot gas [65] predict that erosion proceeds mainly through ejection of C_2 groups following electron collisions and vibrational excitation. As a consequence, the aromatic structure will tend to be preserved throughout the destruction process. Photochemical modeling studies also indicate that under UV irradiation, large PAHs undergo complete dehydrogenation and assume a flexible closed cage structure, which subsequently contracts through the loss of C_2 units until achieving the symmetric C_{60} molecule [66].

The examples regarding the formation mechanism indicate that the formation and evolution of fullerenes and PAHs are interconnected through carbon components such as graphene, graphite, hydrogenated amorphous carbon, soot, and hydrocarbons. This interconnection highlights the necessity of collaboratively studying fullerenes and PAHs within laboratory environments.

1.2.3 Photo-driven evolution

Alongside IR emission, fragmentation acts as a competing process for vibrationally excited molecules. The timescales for these two processes differ significantly. Fragmentation due to photo-driven processes occurs on a timescale of ps, with the loss of H, H_2, or $C_{2n}H_x$ typically dominating the experimental mass spectra of PAH fragmentation. The processes of such photo-driven fragmentation that involve the random redistribution of energy are frequently referred to as statistical fragmentation.

The processing of PAHs in the ISM is largely driven by UV irradiation, which

can affect their size, hydrogenation, and ionisation states [67, 24, 68]. In the laboratory, a number of studies have focused on the first steps of dissociation under the interaction with a single VUV photon [69, 70, 71, 72], showing the loss of H/H_2 and C_2H_2 fragments for standard PAHs. Other hydrocarbon fragments (e.g., CH_3) were reported for superhydrogenated PAHs [73, 74, 75]. More complete fragmentation patterns were obtained in studies using nanosecond laser irradiation at a particular wavelength [76, 77, 78, 79] or continuous irradiation with a Xe lamp [80, 81]. Although these conditions do not mimic irradiation conditions in astrophysical environments, these experiments reveal the most stable fragments upon photoprocessing. In particular, pure carbon clusters [C_{11}^+–C_{15}^+] appear as major fragments in the photoprocessing of PAHs including coronene and dibenzopyrene ($C_{24}H_{12}$), isoviolanthrene ($C_{34}H_{18}$) and dicoronylene ($C_{48}H_{20}$) [81, 77, 78]. This can be easily explained by dissociation proceeding through H/H_2 loss until formation of a pure carbon clusters (e.g., the coronene cation, $C_{24}H_{12}^+$, leads to the formation of C_{24}^+ which further dissociate into smaller clusters).

Once large PAHs have lost all hydrogen, they can isomerize into buckminsterfullerene C_{60} [76], highlighting the significance of top-down synthesis pathways for chemical complexity in space via the sequential removal of hydrogen units and subsequent losses of C_2 units [60, 66]. A recent study by Sundararajan et al. [79] shows the presence of other dissociation channels (e.g., CH loss) in the case of PAHs containing pentagonal rings.

Recent investigations on the photofragmentation of PAH cations [79, 82] confirm photodissociation fragmentation routes that generate bare carbon clusters C_n^+ but also highlight pathways that conduct to the production of hydrocarbon chains $C_nH_x^+$. Photodissociation of corannulene ($C_{20}H_{10}$) and sumanene

($C_{21}H_{12}$) cations and dications revealed similar low mass products, such as $C_7H_3^+$, $C_8H_5^+$, $C_9H_3^+$ and $C_{10}H_5^+$. This finding first suggests that the fragmentation process is independent of the state of charge of a PAH. For coronene, the channels include dehydrogenation via -H and -H_2/-2H loss resulting in $C_{24}H_x^+$ species, fragmentation of the carbon skeleton through -CH loss, formation of the bare carbon clusters C_n^+ (n=11–15) and the hydrocarbon species $C_nH_x^+$ (n=7-–10) containing one or more terminal hydrogen atoms. The mass-spectra analysis revealed two important results; the absence of bare carbon clusters in the low-mass range and the presence of $C_{11}H_x^+$ to $C_{15}H_x^+$ in the high-mass range which contain only one extra hydrogen atom (x=1), whereas the smaller species $C_7H_x^+$, $C_8H_x^+$, and $C_9H_x^+$ exhibit a range of hydrogen atoms (x=1–9). A wide range of smaller hydrocarbons was found in these studies, indicating that these species may represent the end products of the top-down interstellar chemistry of PAHs.

Photodissociation of PAHs has also been explored at higher energies using soft X-rays. In those studies, the photon energy is varied around the innermost electron shell while mass products are analyzed. It was found that above the carbon K-edge, the carbon backbone scission takes over the H/H_2 loss channel [83]. Dehydrogenation will then strongly depend on the photon energy.

1.2.4 High-energy colllisions

Statistical fragmentation of molecules refers to a process in which excess energy causes dissociation pathways once the acquired energy is distributed across various molecular degrees of freedom. The process occurs over a timescale ranging from picoseconds to longer durations. The knockout of individual atoms, such as hydrogen and carbon, due to high-energy collisions with atomic

projectiles, constitutes a non-statistical fragmentation process, as the energy is focused on the ejected atom rather than being dispersed throughout the molecule before the atom's release. Non-statistical fragmentation transpires roughly 1,000 times more rapidly than statistical fragmentation phenomena, occurring on a timescale of femtoseconds (fs).

High-energy collisions represent other key drivers of PAH evolution in astrophysical media through cosmic rays, shocks, and winds. Understanding knockout-driven reactions in high-energy collisions requires an analysis of the energy transfer terms in the interstellar medium, specifically nuclear and electronic stopping. In the collision of individual ions or charged particles with large molecules or molecular clusters, a fraction of the projectile's kinetic energy may be imparted to the target. This may happen under several conditions, such as in laboratory settings, in theoretical models, or within the interstellar medium. The transmission process may originate from either electronic or nuclear stopping. [62, 64]

Electronic stopping refers to the excitation of the electron cloud within the molecular or cluster target. This process is inelastic and serves as the primary mechanism for energy absorption during high-velocity collisions exceeding several hundred kilometers per second. Thus, in electronic stopping, energetic ions engage with the electron cloud of molecules in the ISM, leading to their excitation or ionization. This kind of scattering process leads to a decrease in kinetic energy for the incoming ion and could lead to electronic excitations in the molecule or a statistical fragmentation event.

Nuclear stopping denotes the transfer of projectile energy to target nuclei in Rutherford-type scattering events. The concept was first conceived based on Bohr's research [84, 85]. It is essentially an elastic process comparable to the

collision of solid spheres, where the primary energy transfer mechanism occurs in low-velocity impacts, with speeds approaching several hundred km/s. The absorption of projectile energy can lead to the ejection of individual atoms, a process resulting from nuclear stopping. This phenomenon is exclusive to atom or ion interactions with molecules and does not arise from bombardment by electron or photon projectiles. This process is characterized as non-statistical fragmentation, as the energy is localized to the ejected atom rather than being distributed throughout the molecule. A minimum energy threshold, termed threshold displacement energy, is necessary for the molecule to expel a single atom, which depends on the atomic type and its bonding with nearby atoms. Knockout fragments of molecules are typically more reactive than those produced by statistical fragmentation mechanisms, enhancing effective molecular growth in clusters affected by atomic or ionic projectiles. [86, 87].

In summary, electronic stopping predominates at higher energies, whereas nuclear stopping becomes significant at lower energies and for heavier ions.

The following two sections address two important cases of PAH processing by collisions: cosmic-ray-induced destruction and shock processing.

Cosmic-ray induced destruction

Cosmic rays (CRs) constitute a significant element of the interstellar medium (ISM), substantially enhancing its energy density to 2 eV cm^3 [8]. Cosmic rays mostly comprise relativistic protons, α particles (about 10%), and heavier ions and electrons (around 1%). Concerning the destruction of PAHs, cosmic rays possess two significant attributes: firstly, they can effectively transfer energy to PAHs at energies reaching 10 GeV, potentially resulting in their complete destruction; secondly, they traverse the ISM with near-uniformity and

can penetrate areas like dense clouds, which are otherwise scarcely affected by high-temperature ions and electrons [65].

A few laboratory studies have been conducted to investigate this high-energy interaction. Chabot et al. [88] examined, for instance, the lifetime of free-flying PAHs after their interaction with heavy cosmic rays with the help of theoretical calculations supported by a few validation measurements. Modelling of this mechanism by Micelotta et al. [65] shows that CR processing can be important in weakly shielded environments. Shocks should play an important role in the destruction of PAHs during their journey in the ISM through collisions with fast atoms or ions. Stellar winds, streams of particles that the star expels, represent another source of energetic particles that can alter PAHs. These winds could, for instance, lead to the production of molecular hydrogen H_2 from PAH processing [89].

A limited number of studies have been devoted to investigating the results of high-energy collisions with atomic projectiles. Large facilities, along with a few tabletop experiments, have been employed in this endeavor.

Lawicki et al. [90] investigated kilo-electron volt collisions involving multiply charged ions (He^{2+}, O^{3+}, and Xe^{20+}) and the PAH molecules coronene and pyrene, resulting in the formation of tiny C_nH_x units characteristic of linear-chain molecules. The time-of-flight mass spectrum for the coronene molecule was acquired by bombarding it with protons at energies between 75 and 300 keV. Minor fragmentation peaks $C_nH_x{}^+$ (n = 3 -7) show up in the spectra due to enhanced energy transfer to the molecule. [91].

In the high-energy range (several keV), in which the energy transfer is dominated by charge exchange and electronic stopping, laboratory experiments on the collision of multiply charged ions with small to medium size PAHs,

conducted with heavy ion accelerators and tabletop experiments, have shown substantial fragmentation with the domination of -H, -H_2, and -C_2H_2 losses as well as the formation/ growth of multiply charged fragments [e.g. 92, 90, 89, 93]. The formation of molecular hydrogen (H_2) is a critical initial fragmentation step for internal polycyclic aromatic hydrocarbon (PAH) temperatures over approximately 2200 K, irrespective of the excitation method employed (ions, photons, electrons, etc.) [94].

Studies performed with the help of ion storage rings operating at lower energies in the center of mass (∼100 eV) - in which nuclear interactions dominate - show that in collisions of anthracene ($C_{14}H_{10}$), perylene ($C_{20}H_{12}$) and coronene ($C_{24}H_{12}$) cations with He, non-statistical processes, leading to *e.g.* -CH_x loss or C atom -loss, become increasingly important as the PAH size increases [95, 96, 97]. The prediction is that these mechanisms will strongly dominate the fragmentation pathways for large enough PAHs. The fate of PAHs in shock-dominated regions has been explored through modeling by [64]. In that modeling work, the effects of energetic (0.01–1 keV) ions (H, He and C) and electron collisions on PAHs in interstellar shock waves were examined. It was found that 50-carbon-atom PAHs are significantly disrupted in ionic collisions for shock velocities below 75 km s^{-1}, mainly by sputtering during nuclear interaction.

Shock processing

Throughout the interstellar space, shock waves are ubiquitous. "A shock wave is an irreversible, pressure-driven fluid-dynamical disturbance. The irreversible character is due to entropy generation as ordered kinetic energy is dissipated into heat" [98]. Heat dissipation may vary based on the interstellar medium.

Dissipation in the neutral gas phase occurs due to molecular viscosity during the shock transition, which occurs when there are large velocity gradients and viscous strains. Dissipation in low-density plasmas can be considered collisionless due to the collective motions of the charged particles and the corresponding electromagnetic fields. The dissipation in partially ionized gases can occasionally be attributed mainly to friction related to neutral-ion slip. Irrespective of the dissipative mechanism, shock waves are inherently compressive. The aforementioned dissipation strategies in different media may greatly influence the structure of shock evolution and the emission from the heated shocked gas.

Two types of shocks are of interest in the interstellar medium.[98]

1. J-type shocks: Sometimes referred to as J for Jump shocks, denote a scenario in which the physical conditions (density, temperature, and velocity) demonstrate a sudden transition between the pre-shock and post-shock zones. This is analogous to typical hydrodynamic shocks in physics.

2. C-type shocks: These are referred to as C-type (C for Continuous) shocks, as the physical properties transition smoothly throughout the shock front. This shock condition frequently arises from the interaction of charged matter with the magnetic field and particles that are neutral in a weakly ionized plasma.

Thus, the J-type shocks are characterized by a sudden discontinuity and elevated temperatures, leading to significant molecular dissociation, whereas C-type shocks exhibit a smooth transition, lower temperatures, and diminished dissociation probabilities. (More details about shock waves with shock tubes will be discussed in Chapter 02).

Shocks occur during the creation (jets and bipolar flows; [99]), evolution (stellar winds; [100]), and collapse/death (supernovae and supernova remnants; [101]) of stellar objects (such as stars), as well as in the growth of dense structures (molecular clouds) via convergent flows [102]. It is widely recognized that interstellar dust, which plays a significant role in these environments, experiences profound changes due to shock effects [103, 64, 104, 105, 106, 107]. The specifics of these mechanisms and their magnitude remain inadequately understood. Significant disparities exist between the characteristic durations of grain production in evolved stars and the quick destruction occurring in interstellar shocks [108], particularly for carbonaceous substances [109]. The processes that regulate the evolution of carbon-based grain [106, 107] and also silicates [110] undoubtedly contain numerous ambiguities. A comprehensive knowledge of these shock investigations will enable us to assess their energy, chemical in nature, and star formation effects, and ultimately their significance in the creation and the progression of the interstellar medium (ISM). The identification of the shock product matter is crucial, since determining the nature of the components released in the form of gases may aid in the pursuit of additional chemical tracers for shock events in space.

Shock processing in ISM:

Interstellar shocks typically propagate at velocities between around 1 km/s and many tens of thousands of km/s, depending upon the interstellar region, resulting in post-shock temperatures that fluctuate from several tens of K to 10^9 K [100]. In regions characterized by high-velocity shock waves ranging from 10 to 100 km/s within the low-density interstellar medium (n(hydrogen) < 1 cm^{-3}) and low-velocity shocks in the dense interstellar medium (n(hydrogen) between 10^4 and 10^4 cm^{-3}), knock-on sputtering takes precedence over thermal

processing phenomena [103]. A few examples of low shock velocity propagation in the interstellar medium are provided. Early-type stars can generate shock waves with velocities reaching up to 10 km/s. McKee et al. [111] observed that asymptotic giant branch (AGB) stars are capable of producing shock waves with a Mach number of 6. Shock waves in the circumstellar shells of late-type stars, with shock velocities ranging from Mach 3 to 6, are crucial to the molecular destruction processes [112]. For lower velocity shocks of approximately 1-2 km/s, characteristic of turbulent zones, thermal processing predominates over sputtering, facilitating their investigation in laboratory surroundings, such as through the use of shock tubes.

The Northern Extended Millimeter Array (NOEMA) and the Atacama Large Millimeter/sub-millimeter Array (ALMA) have facilitated comprehensive investigations of the molecular constituents of astrophysical entities, including shock zones. These findings can now be augmented by observations from the recently launched James Webb Space Telescope (JWST), which can investigate shock regions with excellent resolution and sensitivity to carbon molecules. The JWST identifies light within the near-infrared and mid-infrared wavelengths of the electromagnetic spectrum. The instruments cover a wavelength range of around 600 to 28500 nm. Thus, the data obtained in the shock processing experiments can be compared with the observed data.

Shock processing in laboratory studies: Shock tubes can be employed for the thermal processing of gases and materials; they may also function as an alternative to prevalent photon-induced heating techniques for investigating shock processing. Low-velocity shock waves (1-2 km/s) relevant to the ISM can be easily reproduced in the laboratory using shock tubes. Shock tubes have been traditionally utilized in chemical kinetics, combustion, and reentry studies

into the Earth's atmosphere [113, 114]. Few recent studies in astrophysics and astrochemistry are available in the literature on fullerene, organometallic, and amorphous carbon dust particles. The initial studies primarily examined the experimental characterization of changes in carbonaceous analogs, specifically fullerene C_{60}, resulting from shock wave propagation in both the presence and absence of a hydrogen-containing gas mixture [115, 3]. Additional varieties of analogs are now under investigation. Recently, the evolution of organometallic and amorphous dust particles was investigated using low-velocity shock waves[116, 117].

Exploring the scope of shock processing studies in laboratory astrophysics and astrochemistry must include an understanding of both the limitations and the unique advantages offered by traditional shock tubes.

Some limitations of laboratory astrophysics/astrochemistry studies in the shock tubes are listed below.

1. During the shock processing experiments, the pressure increases by several orders of magnitude within microseconds, reaching 30-40 bars, which is significantly higher than the levels found in even dense interstellar regions.

2. The increased collision rate behind the reflected shock wave ensures uniform thermalization and promotes the unimolecular decomposition of the sample in the presence of the surrounding argon bath gas within a laboratory-accessible duration (dwell time). Local thermodynamic equilibrium conditions are easily achieved, unlike those in dense interstellar clouds.

3. In the case of the large solid samples thermalized behind the reflected shock wave, the non-radiative and radiative relaxation of larger and smaller

molecules can lower the actual temperatures below those of the surrounding bath gas.

Despite the preceding limitations, shock tubes offer several advantages over other conventional astrochemistry studies.

1. Shock tubes offer a notable advantage compared to other experimental setups due to their capacity to rapidly raise gas temperature by several thousand Kelvin for durations reaching several milliseconds, followed by a swift quenching process within a few milliseconds. This rapid thermal rise and fall is difficult to replicate with traditional equipment like furnaces and reactors typically employed in similar studies. The rapid heating and quenching act as a common stimulus for the fragmentation or reorganization of unstable molecules at lower temperatures.

2. The shock tube facilities in astrophysics serve as a distinctive apparatus for simultaneously distributing energy to all vibrational modes of a molecule, facilitating the investigation of chemical reactions at elevated temperature and pressure conditions. The facility provides access to a high-energy domain where statistical processes (discussed earlier) are expected to dominate in the interstellar medium.

The uniform energy distribution achieved through collisions in shock processing is essential for large molecules, such as PAHs or fullerenes, to reach high internal energy levels akin to those in low-velocity shock regions of the interstellar medium. This provides us with the opportunity to investigate shock processing research on large molecules, particularly PAHs, in our shock tube facility. Chapter 3 of this thesis will examine the evolution of PAHs during and after the shock processing.

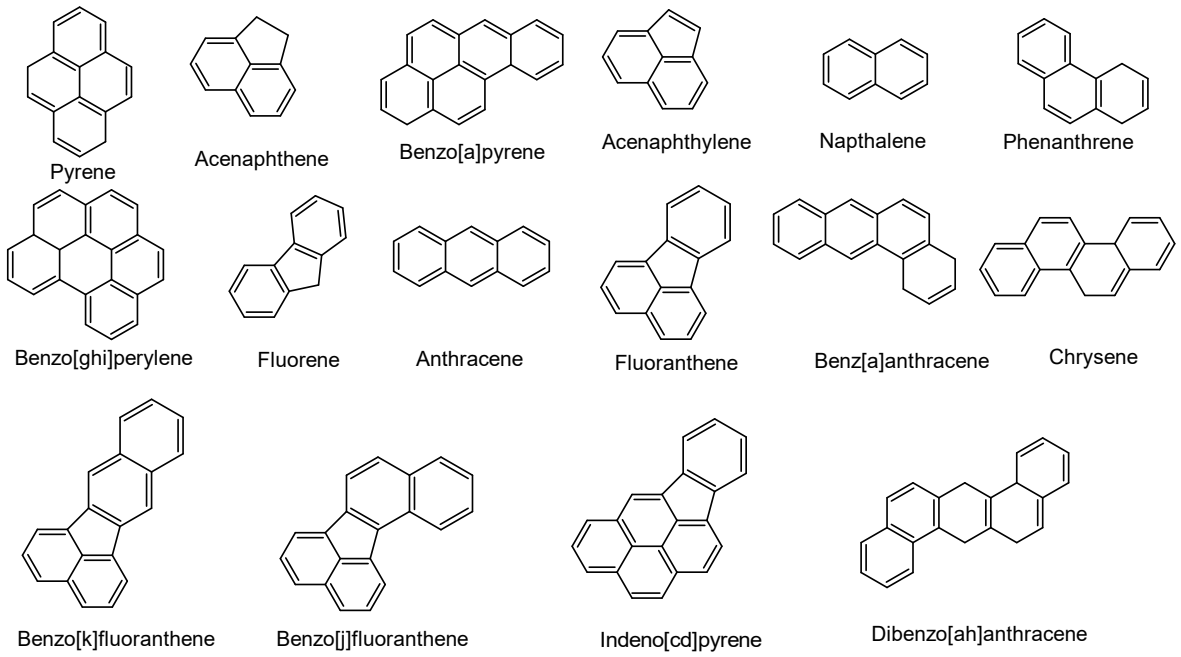


Figure 1.3: The Environmental Protection Agency (EPA) lists 16 priority polycyclic aromatic hydrocarbons (PAHs).

1.3 Combustion

This section of the chapter examines the PAHs on the Earth. PAHs are ubiquitous on Earth, found in the atmosphere, water, and soil.

1.3.1 Observation and formation

PAHs are introduced into the Earth's environment from natural sources, including wildfires, volcanic eruptions, and oil seeps. Man-made sources of PAHs mostly stem from the incomplete combustion of organic materials, including coal, oil, gas, wood, and trash. Secondary sources also include the industrial facilities, vehicle emissions, and household activities, including cooking and heating with solid fuels [118]. PAHs are present even in the remote locations, such as the Arctic snow and ice [119, 120], high-altitude lake deposits [121], and sediments from the deep sea [122]. The origins and environmental behavior of PAHs have been extensively studied due to the harmful properties of some

isomers, necessitating regular monitoring of their quantities and sources. The 16 EPA PAHs (see Figure 1.3) refer to a set of 16 polycyclic aromatic hydrocarbons identified by the United States Environmental Protection Agency (EPA) as priority pollutants due to their potential danger to human well-being. The 16 PAHs are acenaphthene, acenaphthylene, anthracene, fluoranthene, fluorene, naphthalene, phenanthrene, pyrene, benz[a]anthracene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[ghi]perylene, benzo[a]pyrene, chrysene, dibenz[ah]anthracene, and indeno[cd]pyrene [123]. These PAHs are concerning due to their potential toxicity to humans and other terrestrial organisms, as well as their widespread presence and persistence in the environment.

1.3.2 Fuel studies

One of the primary sources of PAHs is the combustion of transportation fuel. Transportation fuel represents about 20% of global energy consumption, with liquid fuels making up 95% of the energy used for transport, primarily sourced from petroleum refining [124]. Different fuel types, such as gasoline, diesel, and jet fuel, are used in engines designed for compression ignition, spark ignition, and gas turbine operations, respectively. Fuels contain many different hydrocarbon species, including n-alkanes (n-paraffins), iso-alkanes (iso-paraffins), cycloalkanes (napthenes), aromatics, alkenes (olefins), and oxygenates. Fuel studies are essential for understanding the formation of PAHs in the Earth's environment.

Types of fuel

1. Gasoline (C_n, where n=4-12): Comprises alkanes including n-butane, isobutane, n-pentane, iso-pentane, and various methyl-substituted hexane,

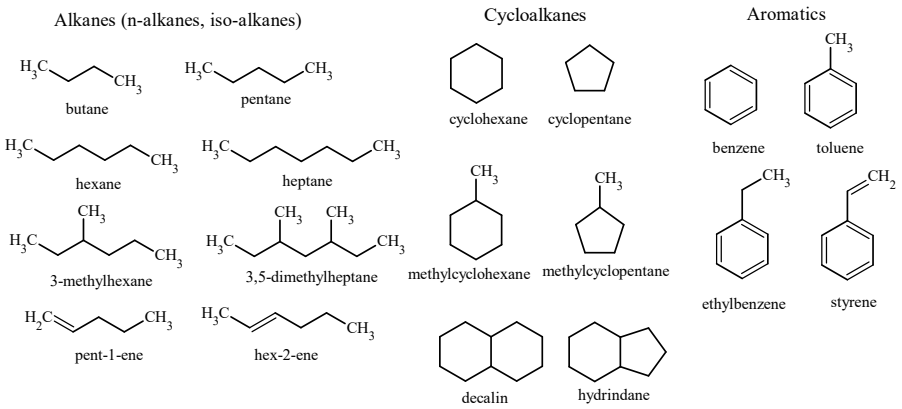


Figure 1.4: Major components of fuel

heptane, and octane. Cycloalkanes present in gasoline generally range from n=4 to n=8, including cyclopentane, methylcyclopentane, cyclohexane, methylcyclohexane, and dimethylcyclohexane isomers. Olefin includes n=5-8 (linear and branched isomers of pentene and hexane). Aromatics: (including benzene, toluene, m-xylene, o-xylene, etc.) [124].

2. Diesel (C_n, where n=10-12): Consists of n-alkane, iso alkane, cycloalkanes (cyclohexane with numerous alkyl side chains), bicyclic and bigger cycloalkane (less than 5% of the total fuel). Aromatics are predominantly monocyclic, such as alkylbenzenes, with a minor presence of substituted bicyclic aromatics, such naphthalene [125]. Diesel is also made from coal. Diesel derived from direct coal liquefaction (DDCL) is composed of approximately 9.3% alkanes, 88.1% cycloalkanes, and 2.6% aromatics by mass [126].

3. Aviation fuel (C_n, where n=8-16): There are various types of jet fuel available in the market, including JP-4, JP-5, JP-7, JP-8, RP-1, and RP-3. (where, JP=Jet Propulsion, RP=Rocket Propellant) [127, 128]. Few are mentioned in the table 1.1.

	RP-1	RP-3	JP-8 (Jet A)	JP-7	JP-5	JP-4
cycloalkanes	58	37.7	20	32	34	29
alkanes	39	53	60	65	45	59
aromatics	3	4.6	18	3	19	10
alkenes	-	2	2	-	2	2
others	-	2.7 (alcohol)	-	-	-	-

Table 1.1: Aviation fuel with composition

Surrogate fuel

The actual fuel consists of hundreds of individual compounds, each present in varying concentrations depending on the specific type of fuel. For practical purposes in modeling and study, particularly in the development of a chemical kinetic model, it is impractical to include all components. The reduced chemical reaction mechanisms are employed to examine combustion processes in conjunction with fluid dynamics in Computational Fluid Dynamics (CFD) simulations. CFD simulations enable direct comparison of real fuel models with experimental facilities concerning their combustion properties across various engines, thereby facilitating conclusions about their combustion behavior. As the number of species increases, the number of reactions also increases, making the CFD calculation more challenging.

To address this issue, we use surrogate fuels as an alternative to conventional fuels. Surrogate mixtures consist of a limited number of components specifically formulated to replicate the physical and/or chemical properties of commercial fuels. A detailed method for developing surrogate mixtures has been outlined by Huber et al. [129]. The two main categories of surrogates are :

1. Physical surrogate: A mixture having the same physical properties, including vaporization, density, viscosity, surface tension, and diffusion coefficient, etc., as the fuel

2. Chemical surrogate: A mixture with similar chemical properties, including flame speeds, ignition characteristics, molecular weight, carbon-to-hydrogen ratio, adiabatic flame temperature, etc., as the fuel

A thorough review of the potential surrogates is provided in the thesis by Hossain et al. [130]. A few examples of surrogates are mentioned here:

- Gasoline surrogates: (Group 1: n-heptane, iso-octane, and toluene [131]) (Group 2: iso-pentane, n-hexane, and methylcyclopentane [132]).
- Diesel : (Group 1: n-decane, iso-octane, methylcyclohexane, and toluene.) (Group 2: n-hexadecane, heptamethylnonane, n-decylbenzene, and 1-methylnaphthalene) [133].
- DDCL: n-hexadecane, iso-cetane, decalin, n-butylcyclohexane, bicyclohexyl, and toluene [126].
- Aviation fuel: JP-4: n-hexane, n-nonane, cyclohexane, cyclooctane, n-heptane, n-decane, methylcyclohexane, decalin, toluene, tetralin, n-octane, n-dodecane, 1-methylnaphthalene, n-tetradecane [127].

Cycloalkanes

Cycloalkanes are components present in all available fuels, in various quantities. Cycloalkanes are prone to producing more intermediates, such as aromatics and polycyclic aromatics, which ultimately contribute to soot formation, compared to acyclic alkanes [134]. Table 1.2 shows various fuel compositions containing cycloalkanes, which include aromatics and alkylated cycloalkanes. The remainder of fuel comprises n-alkanes, branched alkanes, and smaller components such as C4 and C5 hydrocarbons.

Cycloalkane	Gasoline	JP-7	RP-1	DDCL	DDCL	Fuel oil
cyclopentane	15	-	14	-	-	-
cyclohexane	48	64	21	14	85	17
decalin	-	29	39	65	15	31
hydrindane	-	1	5	15	-	5
bicyclohexyl	-	1	-	6	-	29
others	-	5	21	-	-	18

Table 1.2: Different cycloalkane components present in the fuel in percentage.

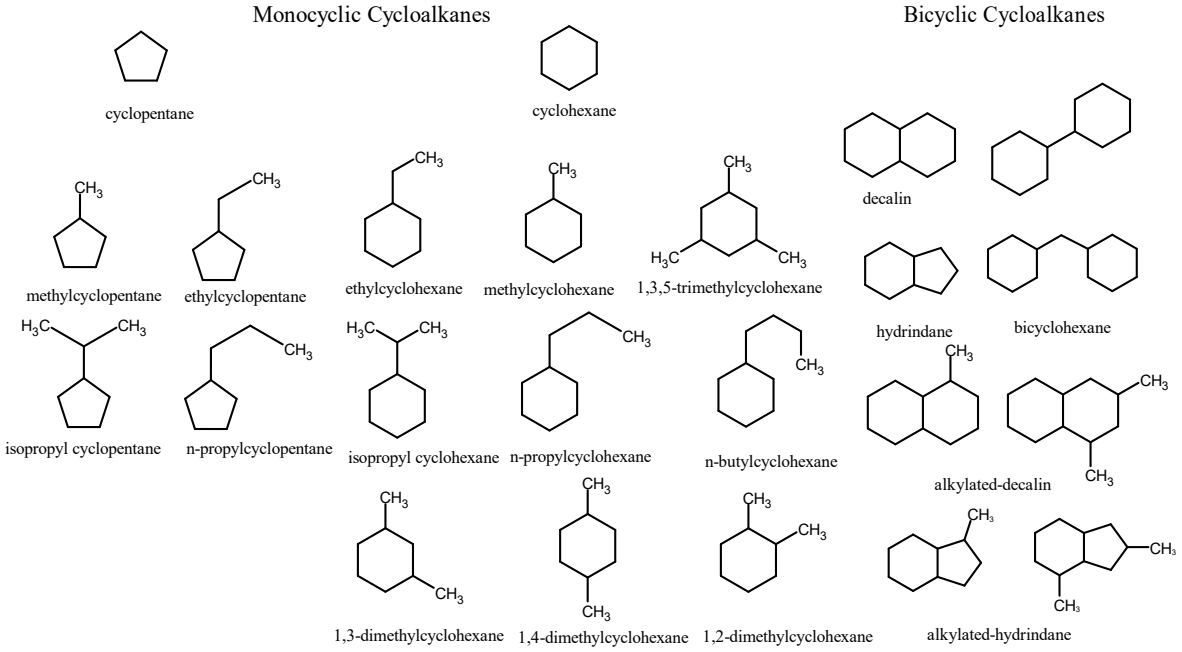


Figure 1.5: Cycloalkanes

The figure 1.5 illustrates various types of cycloalkanes contained in the fuel that could potentially serve as surrogate components. Cycloalkanes generally fall into six groups: cyclohexane, cyclopentane, decalin, hydrindane, bicyclohexyl, and other cycloalkanes (such as cyclooctane and larger). Cyclopentane and cyclohexane are the most studied monocyclic alkanes in the literature, with potential as surrogate molecules. The mechanisms of higher n-alkanes, branched alkanes, alkylated cycloalkanes, and bicyclic alkanes are based on cyclohexane and cyclopentane.

Hossain et al. [130] conducted a comprehensive literature review on alkylated cyclohexane and cyclohexane, confirming that all referenced cyclohexanes in the above figure have been previously investigated. The literature review also reveals that, while cyclohexane and its alkylated derivatives have been thoroughly examined, there is a significant gap in research concerning the cyclopentane derivatives. The existing research on bicyclic alkanes is exclusively focused on decalin, with no investigations conducted on hydrindane. Therefore, in this work, the simplest alkylated cyclopentane and the hydrindane molecule as potential surrogates are examined. A thorough literature review of alkylated cyclopentane, cyclopentane, and decalin has been addressed in the next sections in the table 1.3 and 1.3.3. The following section 1.3.3 will concentrate on the significance of pyrolysis research, including an extensive review of the pyrolysis studies of hydrindane and methyl cyclopentane.

1.3.3 Pyrolysis of fuel

The term pyrolysis originates from the Greek words *pyro*, meaning 'fire', and *lysis*, meaning 'separation'. Pyrolysis of organic materials is a process that involves the breakdown of covalent bonds through thermal degradation in an

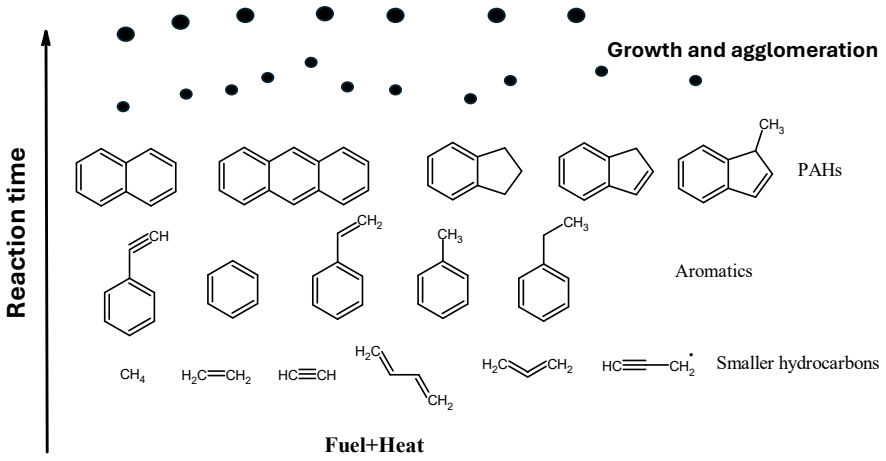


Figure 1.6: Schematic for soot formation via PAHs during the pyrolysis of fuel

inert, oxygen-free environment [135]. Since the major focus of our work is on the PAHs, we chose to study the pyrolysis process. This has certain advantages for aromatic, PAH, or soot formation studies. Pyrolysis is an ideal method for investigating soot production, as the chemical mechanisms of soot formation and growth remain unaffected by the competing oxidation parameters associated with combustion. For eg. during combustion, radicals like O, OH, HO_2, O_2, etc interact with carbon to generate CO and CO_2, leading to carbon depletion.

Why are fuel pyrolysis studies important?

Investigating the pyrolysis of various fuel types, such as gasoline, jet fuel, and diesel, is crucial for understanding combustion mechanisms. These fuels undergo pyrolysis at high temperatures, followed by the oxidation of the resulting smaller species from the initial decomposition processes. The primary goal of these experiments is to reduce soot formation in various combustion processes, particularly in engines, hence enhancing their efficiency. Figure 1.6 shows a simplified schematic of soot formation via PAHs from the pyrolysis of fuel. The thermal decomposition study includes the following steps.

1. Initial decomposition step, including C-H and C-C scission (side chain for alkylated cycloalkanes), in addition to C-C scission for ring opening.
2. Abstraction reactions that include H atom abstraction via smaller radical such as H, CH_3, C_2H_5, etc.
3. The decomposition of cycloalkane radicals yields smaller constituents, leading to the synthesis of aromatic compounds such as benzene and toluene.
4. Rate calculations for all the previously mentioned reactions.
5. Developing a chemical kinetic mechanism based on the available research and the previously mentioned rate calculations.
6. Experimental data collection from various facilities, including shock tubes, flow reactors, etc.
7. Validation of the mechanism through comparison with experimental data.
8. Ultimately, the mechanism can be utilized to gain a deeper understanding of the key reactions involved in the synthesis of aromatics or polycyclic aromatic hydrocarbons (PAHs).

It is essential to note that the rate constants in the literature are often inaccurate for various reactions due to specific reasons.

1. The cleavage of the C-H bond, C-C scission (side chain for alkylated cycloalkanes) and the ring opening (C-C scission) to form an alkene proceed via biradical intermediates and exhibit considerable multireference character.

2. The development of a new pyrolysis mechanism for reactions, including initial decomposition, isomerization, H-atom abstraction, radical decomposition, and other radical chain dissociation reactions, is typically based on estimations derived from analogous molecules.

Therefore, in this work, advanced quantum chemistry computations are conducted to determine rate constants for each of the important elementary reactions.

The next sections will concentrate on the literature to analyze various laboratory and computational studies about the significance of investigating the two chosen cycloalkane surrogates.

Literature review of hydrindane

Bicyclic alkanes are saturated organic compounds comprising two fused or bridged carbon rings that must share a minimum of two common carbon atoms, referred to as bridgehead atoms. Bicyclic alkanes constitute a significant element of fuel, as indicated in the literature review, with additional recent examples provided herein. Bicyclic cycloalkanes constitute the most prominent group of chemicals in the hydroprocessing of pyrolysis fuel oil, accounting for almost 83%. The principal components of the mixture included bicyclohexyl, decalin, methyldecalins, and hydrindane, constituting 28.5, 21.7, 8.7, and 4.2% respectively [136]. Analysis of diesel from direct coal liquefaction (DDCL) indicated that around 80% of the cycloalkanes are also bicyclic alkanes [137, 126, 138].

At present, decalin is the only bicyclic cycloalkane that has been thoroughly investigated through experimental and theoretical methods, particularly in the

Table 1.3: Research on the combustion-related studies of decalin in the existing literature.

Decalin	Experiment	P (atm)	T(K)
[139]	QR pyrolysis (Species analysis)	0.5	973-1223
[140]	Pyrolysis (Species analysis)	1.78	1093
[141]	QR pyrolysis (Species analysis)	1	1053-1073
[142]	FR pyrolysis (Species analysis)	1	973-1123
[143]	TF pyrolysis (Species analysis)	1,2	1083
[144]	TR pyrolysis (Species analysis)	1	1083
[145]	Pyrolysis (Species analysis)	1	770-1020
[146]	FR Pyrolysis (Species analysis)	23-75	698-748
[147]	Reactor pyrolysis (Species analysis)	3.95	1083
[148]	FR pyrolysis (Species analysis)	0.04,0.2,1	920-1500
[149]	FR pyrolysis (Species analysis)	20-100	700-810
[150]	ST oxidation (Ignition delay)	0.6-1.5	1060-1290
[151]	ST oxidation (Ignition delay)	09-48	993-1305
[152]	FR oxidation (Species analysis)	8	600-800
[153]	FR oxidation (Species analysis)	8	626-731
[154]	Motored engine oxidation (Species analysis)	5-17	750-950
[155]	ST oxidation (Ignition delay)	11.7-51.2	769-1202
[156]	FR oxidation (Species analysis)	0.0395	500-2200
[157]	QCC (aromatic formation)	HPL	700-1500
[158]	QCC (H-abstraction reaction)	0.001-100	200-2000
[130]	QCC (thermal decomposition)	HPL	800-2000

context of pyrolysis and oxidation. It is an important constituent in diesel oil, kerosene, jet fuel, and an important component found in of oil shale, oil sand, and direct coal liquefaction [129]. Yue et al. [159] reported that, in an electrically heated tube reactor, hydrocarbons with a higher hydrogen-to-carbon ratio facilitate thermal cracking more efficiently, absorb greater amounts of heat (endothermic cooling), and produce less coke/soot deposits. Hydrogen donor additives restrict the production of multiple thermal soot deposits by supplying H-atoms to the radicals produced during thermal decomposition. Hence, the H/C ratio is a very important parameter for the bicyclic alkane surrogates. This is one of the main reasons why decalin is considered as an ideal surrogate. Consequently, several studies have chosen decalin as a primary surrogate component. A detailed literature review is given in the table 1.3. (where ST = Shock tube, RCM=Rapid compression machine, JSR = Jet stirred reactor, PFS=Premixed flames, LFS = Laminar flame speed, QCC=quantum chemistry calculation, HPL=high pressure limit, FR-Flow reactor, QR = quartz reactor; TF=Tubular furnace; TR=Tubular reactor). A substitute for decalin is essential, possessing comparable chemical and physical properties to function as a viable surrogate molecule.

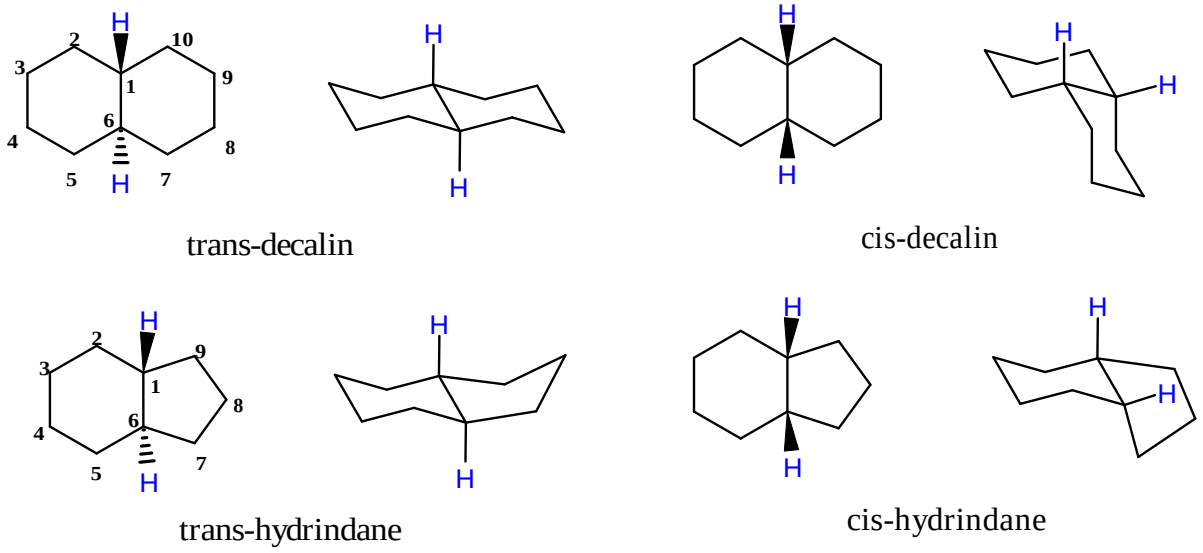


Figure 1.7: Skeletal structure of bicycloalkanes: cis and trans hydrindane, cis and trans decalin.

Hydrindane (C_9H_{16}) is a bicyclic hydrocarbon consisting of a fused cyclohexane ring and a cyclopentane ring. Hydrindane is an important component of JP-7, RP-1 DDCL, and RP-3, as stated in the previous section. Figure 1.7 shows bicyclic alkanes (cis- and trans-hydrindane (C_9H_{16}), cis- and trans-decalin ($C_{10}H_{18}$)). The hydrindanes exist as cis and trans diastereomers (fused ring structure of CH and CP). Whereas cis-decalin and trans-decalin are stereoisomers of decalin, the fused ring structure consists of two CH rings. In cis, both hydrogens are at the bridgehead position on the same side of the molecule, whereas in trans, they are situated on opposing sides. In trans-decalin, both ring junctions are equatorial, resulting in a comparatively flat conformation, but in cis-decalin, one ring junction is equatorial and the other is axial, causing the molecule to assume a tent-like structure. The axial group's A-value is approximately 1.75 kcal/mol. The A-value represents the difference in Gibbs free energy between the higher energy conformation, i.e., the axial substitution, and the lower energy conformation, i.e., the equatorial substitution. Thus, making trans-decalin more stable than the cis-decalin. The

Table 1.4: Major properties of trans-decalin and trans-hydrindane.

Properties	**trans-decalin**	**trans-hydrindane**
Molecular weight	138.2 g/mol	124.2 g/mol
H/C ratio	1.8	1.78
Density	0.9±0.1 g/cm^3	0.9±0.1 g/cm^3
Boiling point	185 °C at 760 mmHg	161.0 °C at 760 mmHg
Vapour pressure	0.7±0.2 mmHg at 25°C	3.0±0.1 mmHg at 25°C
Enthalpy of vaporization	41.0±0.8 kJ/mol	38.1±0.8 kJ/mol
Flash point	57.2 °C	47 °C
Surface tension	29.5±3.0 dyne/cm	29.9±3.0 dyne/cm
Molar volume	158.4±3.0 cm^3	140.7±3.0 cm^3
Refractive index	1.469	1.474

cis-hydrindane exhibits a folded conformation and exhibits a greater enthalpy and entropy of 1.07 kcal/mol and 2.3 kcal/mol, respectively, as compared to the trans-hydrindane [160]. Because of the enthalpy differences and greater entropy of cis-hydrindane in comparison to trans-hydrindane, trans-hydrindane is more stable. Therefore, in both molecules, the trans structure exhibits greater stability than cis because of a lower steric hindrance among the two hydrogen atoms on the bridgehead carbons [161]. The structural parameters indicate that trans-decalin is superior to cis-decalin as a bicyclic alkane surrogate in fuel applications. This is further supported by the studies reported in the literature review.

Table 1.4 presents several key features of trans-decalin and trans-hydrindane, which exhibit similarities and are significant from a combustion perspective [162]. The physical and chemical properties mentioned in the table 1.4, along with prior mentioned structural evidence, indicate that trans-hydrindane, similar to trans-decalin, would be an excellent choice for a bicyclic alkane surrogate. Also, Hydrindane (H/C = 1.78) similar to decalin (H/C = 1.80), may serve as an important hydrogen donor for the reduction of pyrolysis (soot/coke) deposits.

The initial steps of the unimolecular decomposition and ring opening of

cycloalkanes are crucial processes in the pyrolysis and oxidation of the above-mentioned cycloalkanes. For example, the initial steps involve C-H bond scission or ring-opening isomerization, which includes C-C bond scission, leading to alkenes. The experimental rate measurement of the bicyclic radicals, for the decalin and hydrindane radicals and the unstable biradical intermediates, is not easy, and therefore detailed theoretical studies of the initial decomposition channels are very important. The theoretical study of the thermal decomposition of hydrindane and decalin is important due to the lack of detailed theoretical and kinetic modeling data about the pyrolysis of bicyclic compounds. Prior study performed by Chae et al. [157] included only single reference calculations to examine a few reaction mechanisms of trans-decalin decomposition, employing the Rice-Ramsperger-Kassel-Marcus (RRKM) and transition state theory (TST) approaches to determine the high-pressure limit rate constants. The investigations did not concentrate on all the preliminary unimolecular and ring-opening isomerization stages.

Recently, Hossain et al. [130] provided a thorough theoretical analysis of the thermal decomposition of trans-decalin, implementing advanced quantum chemical calculations and TST/VTST methods to derive accurate rate constants for all the major elementary reactions related to the initial decomposition of decalin. No such studies have been done regarding the theoretical investigation of hydrindane. To address this gap in the literature, we perform quantum chemical calculations using TST/VTST methods to get rate constants for each of the elementary reactions associated with the trans-hydrindane (HYD). The new mechanism will be validated through a high-temperature and high-pressure pyrolysis investigation in the shock tubes, as detailed in Chapter 4.

Literature review of methylcyclopentane

Cyclopentane (CPT) is often found in commercial gasoline fuels, diesel, and jet fuels, and can represent the naphthene class in surrogate fuels, including multiple components [163]. The octane rating quantitatively assesses the capacity of gasoline and other fuels to withstand detonation, commonly referred to as engine knocking, in spark-ignition engines with internal combustion. Engines with elevated compression ratios require higher octane number gasoline, as they are susceptible to detonation or knocking. The octane number for five-membered rings (CPT = 101.60, methylcyclopentane (MCP) = 89.30, ethylcyclopentane (ECP) = 67.20, Isopropylcyclopentane (IPCP) = 81.1) is comparatively higher than the six-membered rings (Cyclohexane (CH) = 84, methylcyclohexane (MCH) = 73.80, ethylcyclohexane (ECH) = 46.50, Isopropylcyclohexane (IPCH) = 62.8) [164]. Methyl-alkylated cyclopentane has a higher number than all the cyclohexanes. Due to the above reasons, studying cyclopentane, specifically alkylated cyclopentane, is important. However, experimental data and models of the alkylated cyclopentanes are scarce. Table 1.5 presents numerous studies on CPT, while the research on alkylated cyclopentane is comparatively limited.

Few studies regarding pyrolysis, oxidation, and ignition delay of alkylated cyclopentane are discussed here. Investigations on the kinetics of thermal unimolecular breakdown of methylcyclopentane, methylcyclohexane, ethynylcyclopentane, and ethynylcyclohexane have been conducted at temperatures ranging from 861 to 1218 K utilizing the method of very low-pressure pyrolysis (VLPP) [174]. The results were examined for ring-opening bond fission mechanisms and bond fission to methyl and cycloalkyl radicals. The authors formulated high-pressure rate expressions for the whole decomposition of methyl-

Table 1.5: Research on the combustion-related studies of cyclopentane and alkylated cyclopentane in existing literature, where ST = Shock tube, RCM=Rapid compression machine, JSR = Jet stirred reactor, PFS=Premixed flames, LFS = Laminar flame speed.

Fuel	Exp.	P(atm)	Equivalence ratio	T(K)
CPT				
[165]	ST	7.3–9.5	0.5, 1.0, 2.0	1230–1840
[166]	ST	11–56	0.25, 0.5, 1.0	847–1379
[167]	ST	1.1, 10	0.577, 1.0, 2.0	1150–1850
[168]	ST	13–50	0.5, 1.0, 2.0	922–1316
[168]	RCM	20, 40	0.5, 1.0, 2.0	675–934
[169]	RCM	20, 50	1.0	700–980
[170]	JSR	10	0.5, 1.0, 1.5, 2.0, 3.0	740–1250
[171]	JSR	1	0.5, 1.0, 2.0	900–1250
[172]	LFS	1, 2, 5	0.7–1.6	353–453
MCP				
[167]	ST	1.1, 10	0.577, 1.0, 2.0	1150–1850
[169]	RCM	20, 50	1.0	700–980
[173]	PFS	0.04	1.7	–
[171]	JSR	1	0.5, 1.0, 2.0	900–1250
[134]	JSR	1	0.5, 1.0, 2.0	500–1100
[132]	JSR	1	0.5, 1.0, 2.0	700-1100
ECP				
[169]	RCM	20, 50	1.0	700–980

cyclopentane and proved that their findings supported the idea of a biradical mechanism for ring opening.

Tian et al. [167] examined the ignition delay times of CPT and MCP under identical conditions (low and high pressures) to better understand the influence of cyclic molecular structure and alkyl substitution in ignition chemistry. They validated the mechanism from JetSurF 2.0 [175] mechanism. The results indicated that the high-temperature ignition delay times of MCP were lower than those of CP, as alkyl substitution enhanced fuel breakdown and produced a greater quantity of H radicals, hence increasing the reactivity of the fuel.

Fridlyand et al. [169] studied the low-temperature auto-ignition behaviors of CPT, MCP, and ECP using a rapid compression machine (RCM) (20, 50 bar, and 700–980 K) to investigate the effects of alkyl substitution on five-membered ring cycloalkanes. A comprehensive kinetic model was built to capture the ignition delay times of CPT and MCP accurately. The mechanism for the oxidation of methylcyclopentane at both low and high temperatures is established through analogies with cyclopentane oxidation reactions. They found that the reactivity of MCP was enhanced under low-temperature and NTC (Negative Temperature Coefficient) conditions, whereas the difference in fuel reactivity diminished as temperature increased. So, adding a methyl group to the ring lowers the BDE of the C-C bond, which promotes the thermal decomposition of the fuel. This study also represents the sole investigation of ethylcyclopentane within the combustion environment.

The oxidation of cyclopentane and methylcyclopentane was investigated in a jet-stirred reactor at atmospheric pressure, throughout a temperature range of 900 to 1250 K, for fuel-lean, stoichiometric, and fuel-rich mixtures, with a constant residence period of 70 ms [171]. A detailed kinetic mechanism consisting

of 590 species involved in 3469 reactions was constructed, and the simulation results were compared with the new experimental data. Methylcyclopentane demonstrated higher reactivity compared to cyclopentane under the specified conditions, primarily due to the initiation step that produces cyclopentyl and methyl radicals.

Zhong et al. [134] examined MCP oxidation at atmospheric pressure in a JSR within the temperature range of 500–1100 K with equivalence ratios of 0.5–2.0. A comprehensive chemical kinetic model was developed based on existing literature models. The high-temperature MCP sub-mechanism was primarily developed based on the Dayma model with certain changes, while the low-temperature MCP sub-model was constructed using the Fridlyand model as a foundation. The investigation of reaction pathways indicated that, under high-temperature conditions, the unimolecular decompositions of MCP-producing hexene isomers, cyclopentyl, and methyl radicals are more significant. Subsequently, the same group investigated the application of MCP as a surrogate molecule for naphtha. The surrogate blend for the target naphtha was formulated using the chemical functional group technique, comprising 64.2 mol % iso-pentane, 21.0 mol % n-hexane, and 14.8 mol % methylcyclopentane [132]. Naphtha fuel mostly consists of n-alkanes, iso-alkanes, and cycloalkanes. The primary cycloalkanes in the test naphtha are five-membered ring cycloalkanes, specifically cyclopentane and methylcyclopentane. Thus, the authors chose n-hexane, iso-pentane, and methylcyclopentane to create the surrogate mixture, as C5 and C6 hydrocarbons constitute a significant portion of naphtha.

The earlier reported mechanism includes high-temperature pyrolysis and oxidation reactions of MCP, which include unimolecular decomposition, ring-

opening isomerization, hydrogen abstraction, β-scission, and hydrogen migration. The rate coefficients for the initial decomposition pathways of C–C in MCP were determined by drawing analogies with CPT or methylcyclohexane (MCH) reactions. The rate constants of these initial reactions were based on certain assumptions. The rate constant for MCP ring opening is based on CPT, since the activation energy for ring-opening reactions of MCP was assumed to be equivalent to that of CP, given the similarity of the ring structure (ring strain energies for CPT and MCP are 7.1 kcal). The rate constant for the unimolecular decomposition producing the methyl and cyclopentyl radicals was based on MCH, assuming the MCP and MCH have similar bond dissociation energies for the C–C bond between the methyl group and the cycloalkane. Similarly, the rate constants for H-atom abstractions are based on MCH only. The lack of clarity and inadequate knowledge about the unimolecular reactions of MCP require further investigation to analyze the competition between unimolecular decomposition and various ring-opening isomerization pathways. The new mechanism must be validated against the experimental data, which will be achieved through a high-temperature and high-pressure pyrolysis investigation in the shock tubes, to be discussed in Chapter 5.

1.3.4 Laboratory studies of combustion in Shock tubes

The shock tube setup for chemical kinetic studies is essential for the development and validation of chemical-kinetic reaction mechanisms utilized in simulating combustion processes in aerospace ramjets, scramjets, rocket combustion chambers, jet engines, and various other ground vehicle engines.

Key experimental parameters include pressure, temperature, and reaction time, which are essential for carrying out chemical kinetic studies and can

be manipulated in the shock tube facility. Combustion investigations in a shock tube include pyrolysis, oxidation, ignition delay, laminar flame speed assessments, high-speed camera visualization, and soot creation, among others. The analysis of the mechanisms associated with PAH and the subsequent soot production from a fuel, resulting from the pyrolysis of gaseous hydrocarbons, is also achievable due to the uniform pressure and temperature conditions that exist behind reflected shock waves. The combustion diagnostics for shock tubes primarily involve in situ investigation using optical spectroscopy and gas sampling, supplemented by various post-shock analytical techniques for gaseous and solid soot products, if applicable. Optical spectroscopy typically includes emission and absorption spectroscopy methods, while species analysis uses the gas chromatography method. Additionally, recent years have seen the incorporation of shock tubes alongside traditional laser techniques (emission, absorption, and scattering measurements across various spectral ranges), novel techniques such as laser-induced incandescence (LII), laser schlieren densitometry, time-of-flight mass spectrometry (TOF-MS), etc. More details can be found in the review papers on shock tubes. [176] and [177].

GC technique

The detection of gaseous products in shock tube investigations relies on gas chromatography (GC) techniques. GC analysis offers several advantages, including high sensitivity (ppm level detection), exceptional separation efficiency, diversity, and quick interpretation capabilities. These features facilitate a detailed analysis of complex post-shock hydrocarbon mixtures, enabling the identification and quantification of various gases with differing mass and vapor pressures present in the process. The main advantage of different gas chromatography techniques lies in their incorporation of various detectors, including

flame ionization detection (FID), mass spectrometry (MS), thermal conductivity detection (TCD), Electron Capture Detector (ECD), Nitrogen-Phosphorus Detector (NPD), and Flame Photometric Detector (FPD), etc. [178] The identification of reaction products is achieved by comparing retention times with those of known pure chemicals in a complex reaction mixture. Depending on the detector used, such as GC-MS, the structure of products can be identified, while GC-FID allows for the quantification of these products. Certain research groups employ new GC*GC [179] setups and specialized techniques such as time-of-flight mass spectrometry, in conjunction with shock tubes [180, 181, 182], to examine combustion products.

Finally, this study employs a shock tube in conjunction with gas chromatography (GC) methods, as detailed in Chapter 2, Section 2.1.1, and Section 2.2.4.

1.4 Thesis structure

This section provides a concise overview of the introduction, highlighting the key connections between chapters and the overall framework of the thesis. It is crucial to highlight the connection between astrochemistry and combustion investigations, which will be demonstrated through analogous experiments, despite some variations in temperature and pressure across different experiments. The introduction also aimed to emphasize the significance of fundamental combustion concepts for the advancement of astrophysics and astrochemistry, particularly through analogous studies related to PAHs. For instance, research on aromatics, PAH, and soot nanoparticles on Earth overlaps with the astrophysical creation of big carbonaceous molecules and microscopic particulates, or stardust, through PAH evolution.

The thesis is organized into two parts for better understanding: astrochemistry and combustion. The astrochemistry section will address the destruction of PAHs under shock conditions, while the combustion section will focus on the formation of aromatics that ultimately contribute to PAH formation. The shared feature in the study pertains to the pyrolysis conditions achieved in the shock tube facility, a crucial tool for the evolution of PAHs, specifically their formation and destruction. The shock conditions present in the interstellar medium can be considered analogous to those observed in laboratory settings, albeit with certain limitations, as previously mentioned in the chapter. This endeavor aims to connect the two research streams through shock tube investigations. Given that our primary emphasis is on PAHs, we opted to investigate the pyrolysis in combustion in a manner similar to astrochemistry studies. Pyrolysis is an ideal technique for examining aromatic compounds, PAHs, and soot production, as the chemical mechanisms of soot formation and growth are not influenced by the competing oxidation mechanisms related to combustion.

To summarize our literature review, we have established a few important points in both areas:

1. *Astrochemistry:* The significance of coronene as a prototypical PAH, accompanied by observations, formation, and evolution processes in ISM, and the identification of research gaps in shock processing studies, supports the present study in astrochemistry.

2. *Combustion:* The significance of cycloalkanes in the formation of PAHs, which involve both monocyclic and bicyclic alkanes as surrogate compounds in fossil fuels, along with the recognized research gap, supports the current study on combustion.

The thesis structure is as follows, addressing the questions and links mentioned above.

Organization of the thesis:

1. **Chapter 1: Introduction**

   Introduction, literature reviews, and motivational aspects of the thesis for both astrochemistry and combustion studies. This chapter examines the occurrence of PAHs on Earth and in space, highlighting their significance and the justification for investigating PAHs in the context of both astrochemistry and combustion.

2. **Chapter 2: Experimental and Computational Methods**

   Experimental and computational methodologies, detailing the experimental shock tube facilities and computational methodologies. To explore our hypothesis, we will use unique, home-built shock tube facilities in our lab for both studies. This chapter of the thesis examines the specifics of the shock tube facilities, emission spectroscopy tools, gas chromatography instruments, and the computational methodologies employed in this thesis for the study of both topics.

   The astrochemistry experiments include soot samples collected from the post-shock analysis of PAH pyrolysis. However, in the pyrolysis studies related to combustion, with very low fuel concentrations, 2 ms of dwell time, temperatures below 1600 K, and pressures under 25 bar, soot particles are not present. Hence, the combustion experiments focus on data obtained from shock tube experiments in the gas phase, specifically examining the formation of aromatics during gas-phase pyrolysis processes.

3. **Astrochemistry: Chapter 3: Shock processing of coronene.**

This chapter of the thesis examines the shock processing of the coronene supported by other components such as corannulene ($C_{20}H_{10}$), fullerene (C_{60}), fullerene (C_{60}) with hydrogen and ethylene (C_2H_4). This study highlights the use of time-resolved emission spectroscopy for analyzing small components during the shock processing, with findings further supported by ex situ analysis of solid residues and molecular dynamics simulations.

4. **Combustion: Chapter 4: Unimolecular decomposition of hydrindane and Chapter 5: Unimolecular decomposition of methyl cyclopentane**

   This part of the thesis will examine the decomposition of surrogates for bicyclic alkanes and alkylated cyclopentanes. The work is focused on the following points.

   (a) Development of a chemical kinetic model for the surrogates.

   (b) Generation of experimental datasets from shock tube experiments for the surrogate.

   (c) Validation of the model with the experimental datasets.

   Once a kinetic model is validated against experiments, a deeper understanding of the initial decomposition pathways of fuel consumption and the mechanisms leading to aromatic formation can be gained, which ultimately contributes to soot formation.

5. **Chapter 6: Conclusion and future perspectives**.

   The final Chapter 6 consists of a summary of the thesis, highlighting the significant contributions made in each section, key findings, and future perspectives.

Chapter 2

Experimental and Computational methods

2.1 Shock tube

A shock tube is a device recognized for its ability to produce high temperatures and pressures for brief intervals, often lasting from several microseconds to a few milliseconds. Consequently, it is regarded as a millisecond high-temperature furnace for chemical kinetics. The temperature range for investigating the reaction can be considerably increased beyond that of the conventional reactor (1000 K) without the wall effects associated with a flow reactor or furnace configuration. Thus, a shock tube facilitates the investigation of a chemical reaction or process at a certain temperature, free from the effects of surface reactions, secondary reactions, or phenomena happening at intermediate temperatures up to 10000 K and pressures in excess of 100 atm [114].

High-enthalpy shock tube experiments are frequently employed to investigate aerodynamic and chemical kinetic phenomena. The simple bursting-diaphragm technique in a single-pulse shock tube is frequently employed for

studying high-temperature and pressure processes related to homogeneous or heterogeneous gas dynamics. The shock tube is divided into two sections, separated by a thin metal diaphragm. The driver section is filled at high pressure with a low-density driver gas, usually helium. In contrast, the driven section is evacuated and filled at a lower pressure with the experimental gas or the test gas mixture to be studied. When the diaphragm bursts, by raising the driver-gas pressure, the driver gas rushes out into the driven section and produces a shock wave into the driven gas. Upon reaching the end of a shock tube, the incident shock wave is reflected into the gas that has already undergone heating due to the compression of the incident wave. Consequently, the gas undergoes further compression, resulting in increased temperature, pressure, and density.

The process is illustrated in Figure 2.1 by an x-t diagram, which also illustrates the region in which the experiments take place. The vertical axis represents the time that has transpired since the diaphragm rupture, while the horizontal axis represents the position along the shock tube. The reflected shock increases the temperature and pressure of the sample molecules near the end flange till it encounters the reflected expansion wave. The expansion fan encounters the reflected wave prior to reaching the contact surface, leading to a reduction in temperature and pressure. The location near the endwall, situated at the far right in the x-t image, provides ideal conditions for experiments conducted under elevated temperatures and pressures. Various types of pressure sensors, optical detectors, and visualization techniques can be employed in this region to investigate chemical kinetics, spectroscopy, flow imaging, and other related studies.

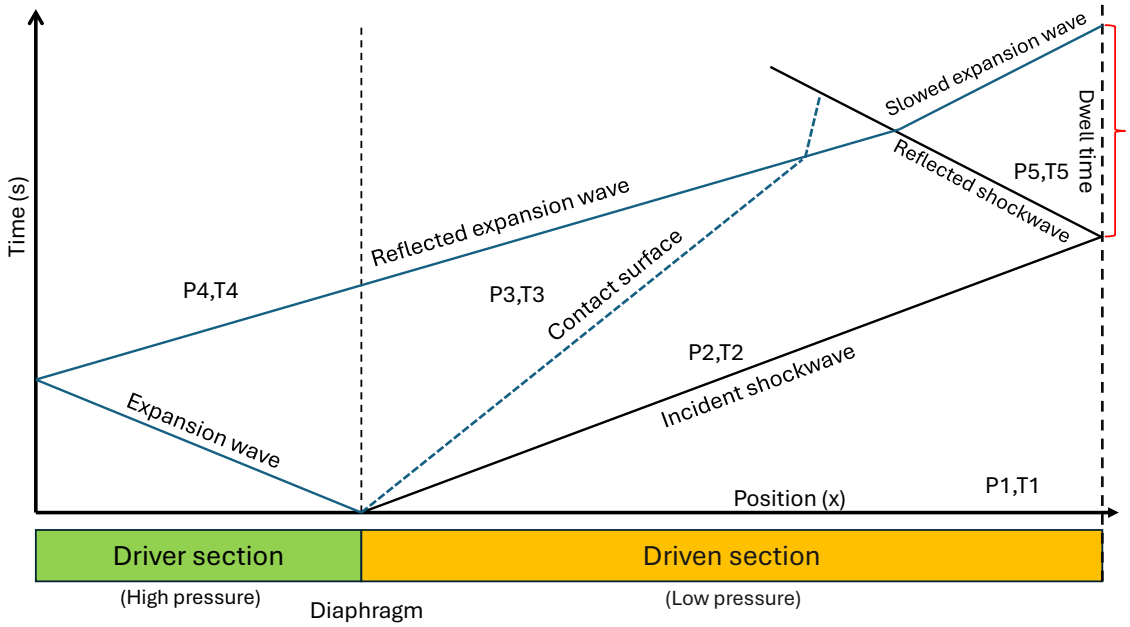


Figure 2.1: The x-t diagram illustrates the propagation of shock and expansion waves within a conventional shock tube. The figure shows a specific condition where the expansion fan meets the shockwave before the contact surface.

According to the convention, the pressure and temperature in various regions are represented as follows: P1, T1 in the initial low-pressure-driven region; P2, T2 in the area between the shock front and contact surface; P3, T3 in the region between the contact surface and expansion wave; and P4, T4 in the high-pressure driver region. Upon reflection of the shock wave at the tube's end section, both temperature and pressure rise, designated as P5 and T5, respectively.

The test time is determined by the interval between the reflection of the shock wave and the arrival of the expansion wave at the end wall, which is a few milliseconds. The duration of the test time/dwell time can be extended by delaying the arrival of the expansion fan through the elongation of the driver section or by slowing the expansion wave by reducing the sound speed of the driving gas through the incorporation of heavier gases in the driver section. More details can be found in the paper "Strategies for obtaining long constant-pressure test times in shock tubes." [45].

The advantages of a shock tube are that the slice of shock-heated gas is very uniform, and the boundary layer at the shock tube wall is usually thin with negligible wall effects. The heating process of the driver gas occurs on the microsecond scale and initially takes the form of high translational energy, which is then converted by collisions to rotational, vibrational, electronic, and chemical forms. In experimental chemical kinetics and spectroscopy studies, the rate parameters are functions of pressure and temperature. The experimental gas can be heated to the required temperature and pressure using the appropriate pressure ratio across the diaphragm or by varying the thickness and grooving of the diaphragm [183].

All physical properties related to the incident and reflected shock waves can be readily calculated from the thermodynamic properties of the shocked gas and the measured velocity of the incident shock. The governing equations for shock wave theory can be expressed by the Rankine-Hugoniot equations, which define the variations in pressure and temperature across a shock wave, depending upon the thermodynamic parameters of the experimentally determined incident shock velocity. Typically, the temperature and pressure behind the shock wave are determined using the formulae presented below.

$$\frac{P_5}{P_1} = \frac{(2\gamma M^2 - (\gamma - 1)}{(\gamma + 1)} \frac{(3\gamma - 1)M^2 - 2(\gamma - 1)}{(\gamma - 1)M^2 + 2}$$

$$\frac{T_5}{T_1} = \frac{[2(\gamma - 1)M^2 + (3 - \gamma)][(3\gamma - 1)M^2 - 2(\gamma - 1)]}{(\gamma + 1)^2 M^2}$$

where M = Mach number (U/a), γ = heat capacity ratio, U = Shock velocity, a=sound speed $\sqrt{\gamma RT}$, R = Gas constant.

2.1.1 Chemical Shock Tube (CST) facility

A single-pulse shock tube facility, the Chemical Shock Tube-1 (CST) with a dump tank [184, 185, 130] was used to conduct the combustion experiments described in this study. The CST facility in our laboratory has been recently upgraded with remote operation capabilities for the shock tube and a new data acquisition (DAQ) system. The facility has undergone significant enhancements, including the installation of two new pneumatic ball valves from PHBB Valves Private Limited, Pune. The two valves have replaced the previously used manually operated ball valve located adjacent to the test section in the driven section, and the filling valve employed to rupture the diaphragm in the driver section. The above-mentioned modifications require the recalibration of the shock tube facility due to the alteration in the shock tube's length, ensuring accurate calculation of the experimental reflected shock temperatures. The CST comprises an aluminum tube with a 50 mm internal diameter and 25 mm wall thickness. The length of the driver section is 1.8 m, and that of the driven section side is 3.3 m. The ball valve is positioned in the driven section, 0.4 m from the end flange, known as the sample chamber or reaction chamber. This method is commonly referred to as the constrained reaction volume (CRV) strategy. A dump tank with a diameter of 100 mm and a length of 2 m is connected near the diaphragm station in the driven section at an angle of 45° to the shock tube. The experiment used an aluminum diaphragm of 1-2 mm thickness and variable grooving for bursting.

2.1.2 Material Shock Tube (MST) facility

We recently set up the Material Shock Tube (MST) facility at the Indian Institute of Science, Bangalore, Laboratory for Hypersonic and Shock Wave

Research (LHSR) Laboratory to study how shockwaves interact with solids and gases in ways that are relevant to astrophysical conditions. The MST comprises a stainless-steel (SS) tube with a 53 mm internal diameter and 25 mm wall thickness. The length of the driver section is 2.1 m, and that of the driven section side is 4.75 m before the pneumatic ball valve. The driver section's length can be altered to provide the appropriate reaction/dwell time behind reflected shock waves. About 2 ms of dwell time was achieved with the 2.1 m-long driver section. The driven section has been divided into two sections by placing a ball valve before the sample chamber/test section. The sample chamber consists of part of the driven section after the ball valve, the sample holder, the extension part, the optical chamber, and the end flange. The sample chamber, the optical flange with lens holders, and the end flange have been made from aluminum to avoid the surface contamination present in the case of SS. A dump tank with a diameter of 100 mm and a length of 2 m is connected near the diaphragm station in the driven section at an angle of 45^0 to the shock tube. The experiment used an aluminum diaphragm of 1-2 mm thickness and variable grooving for bursting.

2.2 Instrumentation

2.2.1 Data acquisition system (DAQ)

The two facilities have independent dedicated DAQ systems that can function independently from the main control panel (see fig. 2.2 and 2.3).

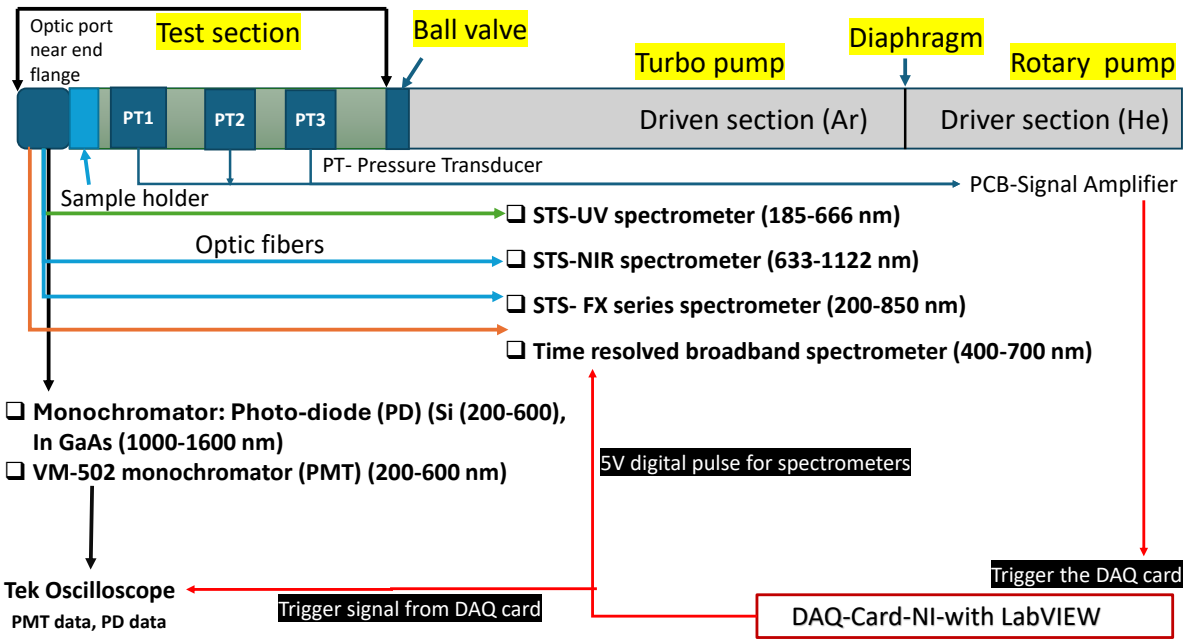


Figure 2.2: Shock tube facility—schematics with instrumentation

For CST- The DAQ system comprised a National Instruments System (NI-PXIe-1071 chassis with NI PXIe-8360 data card and 16 Channel TB-2706 terminal), a Tektronix oscilloscope (model TDS-2014B), three PCB pressure transducers (model 113B22 with 1 mv/psi), and three PCB signal conditioners (model 482A21). The DAQ is linked to a dedicated CST-1 personal computer, which utilizes the GUI-based NI LabVIEW software to manage the entire system.

For MST- The data acquisition is handled by a National Instruments System (USB-6356 DAQ card) and a Digital Storage Oscilloscope (Tektronix-model TBS 2000B series). It reads the output of 3 PCB pressure transducers (PT1, PT2, and PT3 sensors model 113B24 with 5 mV/psi) through PCB signal conditioners with amplification (model 441A42) as well as static pressure gauges and indicators. The DAQ is connected to a dedicated personal computer, where the GUI-based NI LabVIEW software can monitor the whole system.

The pressure sensors are flush-mounted on the shock tube and are connected to the DAQ system by the low-noise coaxial cables via a signal conditioning box acquired from PCB Piezotronics, Inc. The NI-DAQ and the Tek oscilloscope are triggered by the PCB sensor mounted in the shock tube's driven section to obtain the pressure profiles. The pressure profiles of the shock tube are acquired using PCB pressure transducers positioned at designated sites within the driven section (closer to the end flange). Figure 2.4 shows the pressure profile of the CST and MST facilities. Ideal shock temperature has been determined using the normal shock relation, utilizing the measured Mach number (incident shock velocity) using the Wisconsin Gas Dynamics Calculator [1]. The NI-DAQ card triggers the STS-UV spectrometer and the NECTA Line Scan Camera (high-speed CMOS camera) by sending a 5 V TTL pulse. The IRA pressure gauge instrumentation is utilized to fill and monitor the gas fill pressure in the driver or driven section.

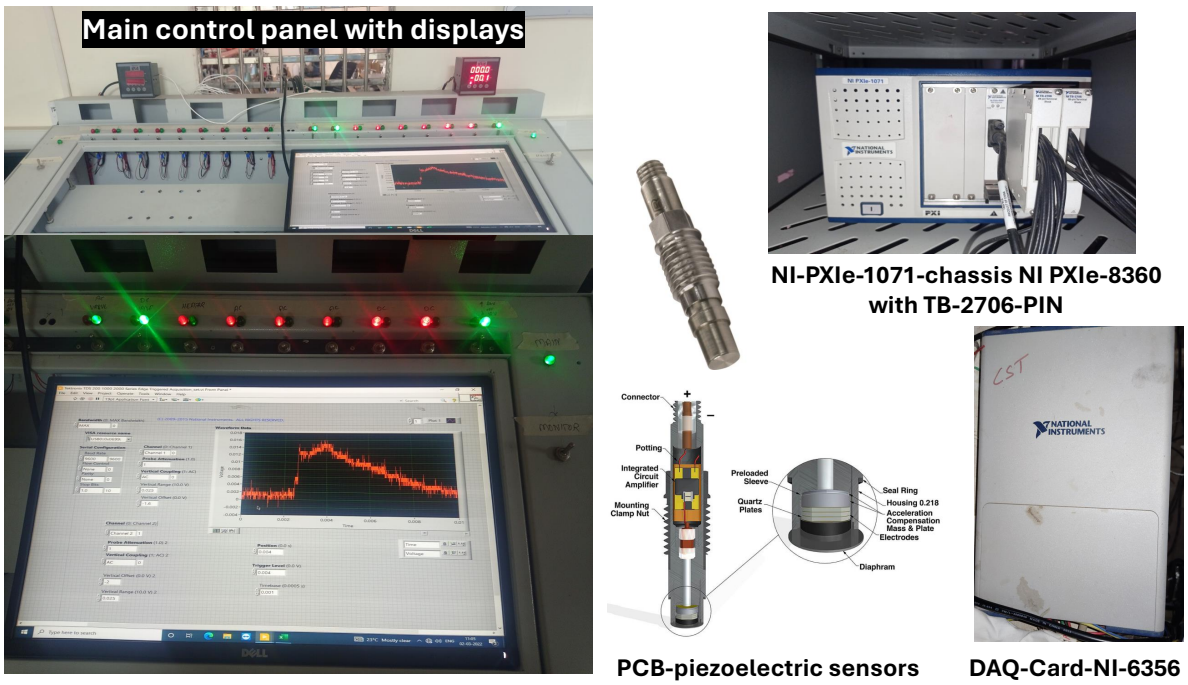
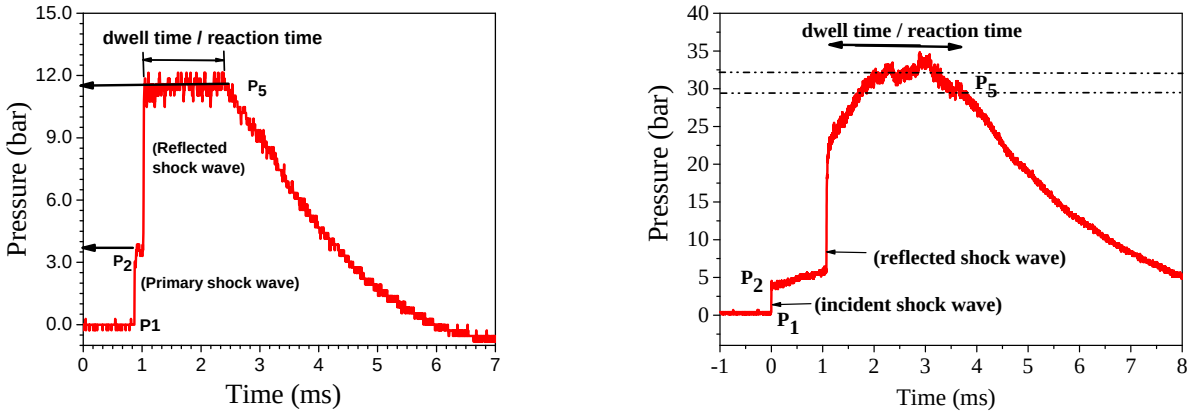


Figure 2.3: NI DAQ description with main control panel for MST and CST facility showing pressure signal from PCB piezolelectric sensors.

[1] https://silver.neep.wisc.edu/~shock/tools/gdcalc.html



(a) (b)

Figure 2.4: Typical pressure trace vs time measured in the sample chamber of the shock tube facility. The curve shows a two-staged sudden rise in pressure with the arrival of the incident shock wave in the driven section and the arrival of the reflected shock wave from the end flange and thereafter a gradual fall in pressure caused by the expansion wave. (*a*) Pressure traces from the CST facility (5 mm from the end flange). Because of the short distance from the end flange, the incident shock front is barely distinguishable. (*b*) Pressure traces from the MST facility (460 mm from the end flange). This figure shows clearly the incident and reflected shock wave.

Dump tank in the CST and MST facility

The dump tank significantly influences reflected shock. The benefit of the dump tank is that it ensures the shock tube has a single-pulse characteristic, hence eliminating multiple reflections within the tube. Further information regarding the mechanism of the ball valve and the dump tank is available in papers (see. [184, 185]). Figure 2.5 illustrates that multiple reflections will further elevate the temperature and pressure of the test gas.

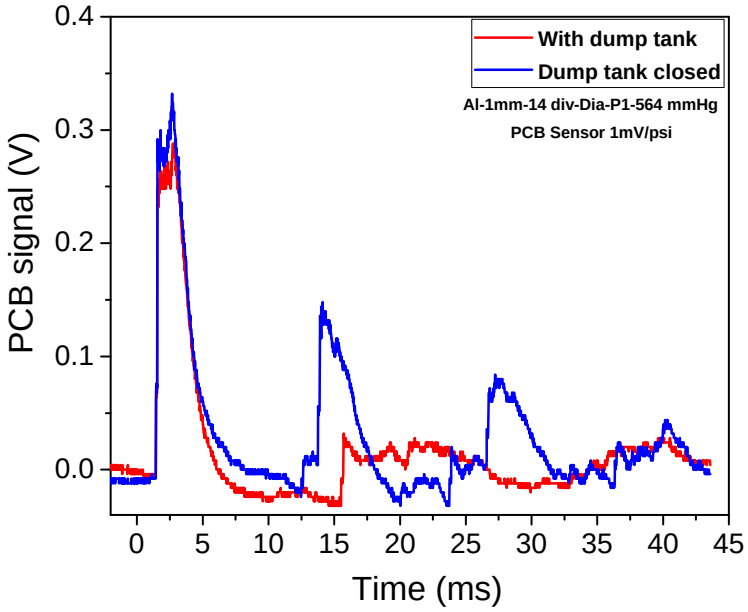


Figure 2.5: P_5 signal at 0.5 mm from the end flange taken under the same experimental conditions to show the effect of the dump tank on pressure signals near the end flange.

In reactions involving radicals, it is not accurate to state that the reaction is quenched due to the absence of a single pulse characteristic. In Rajakumar's work [184], only HF/HCl are present, which implies that the overall reaction exhibits a higher activation energy, preventing repeated reactions. Meanwhile, hydrocarbon experiments involve numerous smaller components and radicals that exhibit lower activation energy compared to the parent fuel or molecule. The abstraction reactions involving methyl, hydrogen, and ethyl radicals exhibit low activation energies, which might be affected by the secondary pressure and temperature rise.

2.2.2 Optical instrument setup

The optical chamber/flange has been explicitly designed to study the in-situ emission spectroscopy in the shock tube in both the CST and MST facilities 2.2 and 2.6. The emission from the shock tube is captured axially along the

tube near the end flange (15 or 5 mm from the end flange) along with the PCB pressure transducer data to get accurate and real-time emission and pressure information simultaneously. The optic chamber has four ports: three are used for acquiring emission, and one has a PCB pressure transducer for pressure signal. The three optical ports collect the emission from the shock tube through a 6.35 mm diameter sapphire half-ball lens from Edmund Optics, and the light is guided to the various optical instruments by optic fibers of different dimensions. The in-house time-resolved spectrometer with high-speed CMOS camera with 1000 µm optic cables; the VM-502 (Vacuum Monochromator) or Mini monochromator series with 200 µm; and the STS Ocean Optics micro-spectrometers with 50 µm (fig. 2.7). All optical instruments are triggered by the incident shock wave so as to cover maximum duration of the shock processing event of around 10 ms.

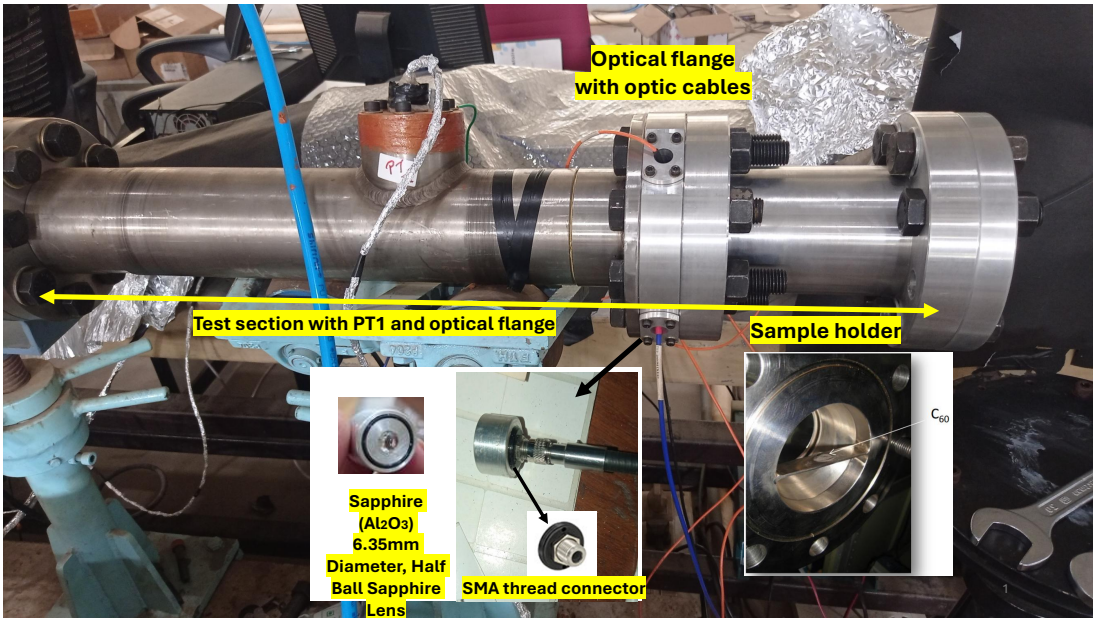


Figure 2.6: MST facility—test section with pressure ports, optical port with optical cables, and sample holder.

Figure 2.7: Optical systems are used for emission spectroscopy studies in the MST and CST facility. *(Figure taken from the references cited in the description.)*

1. *VM 502-(Vacuum Monochromator):* The Acton VM-502 monochromator from Princeton Instruments covers a wavelength range of 30 nm to 600 nm and consists of a DA-780-VUV (PMT-photo multiplier tube) detector, which has a wavelength range of 200 nm to 600 nm . The current configuration consists of an input slit, a concave holographic grating (H-UV blazed) with a groove density of 1200 grooves/mm, an output slit, and the PMT detector. Standard bilateral slits with an adjustable range of 5 micrometers to 3 millimeters are provided. A precise micrometer, graded in increments of 10 micrometers, allows for slit adjustment in a vacuum. It is possible to change the slit height from 0 to 20 mm, depending on the experiment. Vacuum valves are supplied for experiments in the high-vacuum ultraviolet region to separate the slit chambers from the main instrument chamber containing the gratings. The monochromator monitors the emission signal at the given wavelength (such as 510 nm) with respect to time.

2. *Manual Mini-Chrom Monochromator*: The Manual Mini-Chrom Monochromators from Edmund Optics operate within a wavelength range of 190 nm to 650 nm and include a high-speed Si photodetector with a wavelength range of 200-1100 nm. Manual Mini-Chrom monochromators are instruments that have manual operation, utilizing a dial-type operation for wavelength selection. A set of slits with dimensions ranging from 100 to 300 microns is included. The Mini-Chrom is a compact, in-line design based on the Fastie-Ebert configuration. The dial's revolution induces, through a precise lead screw and sine bar procedure, the rotary motion of the diffraction grating, thereby aligning the selected wavelength at the exit slit. The wavelength of the light can be determined in nanometers (nm).

3. *Ocean Optics spectrometer STS and FX series*: The spectrometers have a broad wavelength range, which provides different time and wavelength resolutions. The miniature spectrometers STS-UV and STS-NIR are each equipped with a photodetector array and operate within the wavelength ranges of 186 to 666 nm and 670 to 1100 nm. It demonstrates a resolution of 1.4 nm, dependent upon the slit size, a signal-to-noise ratio greater than 1500:1, and a dynamic range of 4600:1. The miniature spectrometers of the Ocean FX-UV-VIS series operate within the wavelength ranges of 200 to 850 nm. The FX series spectrometer includes an option for modifying slit openings to enhance resolution. The optical emission spectra that were measured are the result of integrating signals over 5 to 10 milliseconds to make sure that the whole shock process of the sample was covered [186].

4. *Time-resolved broadband emission spectrometer (TR-BES)*: The setup includes a manual monochromator and a high-speed CMOS-camera. A

home-built spectrometer disperses the emissions from the shock-heated reaction mixture, and a CMOS line camera records the temporal data of the spectrally resolved emission.

It is composed of a Newport 77250B-MC with a 77298 grating assembly [187], ruled with 1200 lines/mm, 360 nm blaze, to operate in the 200-1000 nm wavelength region. The opening slit can be finely adjusted with a width that can vary from 4 μm to 3 mm and a height that can be adjusted between 2 and 12 mm. The design is derived from the Ebert-Fastie concept, employing a single large spherical mirror to collimate point light entering the input port and to concentrate the diffracted light from the grating at the output port. A resolution of up to 0.1 nm is achieved with the current grating. The central wavelength is chosen by manipulating a manual wavelength selector on top of the monochromator. The exit slit is removed and replaced by a line scan monochrome camera (Sensor type Mono Sensor resolution 1(H) x 4096(W) with a pixel size of 3.5 μm $\times$ 3.5 μm – Alkeria Necta N4K-7). The maximum time resolution that can be attained is 10.6 μs.

5. *High-speed photodetectors with monochromators:* The 818-BB-27 High-Speed UV-Enhanced Silicon Optical Detector is equipped with a silicon detector that is optimized for response across ultraviolet, visible, and near-infrared wavelength ranges. The detector possesses a functional sensor of 2.55 mm and a rise period of 3 ns, functioning within a wavelength spectrum of 200 to 1100 nm. The detector employs a 24 V DC external power supply to attain swift response times. The 818-BB-31 High Speed Photodetector features a free-space InGaAs detector, optimized for wavelengths ranging from 1000 to 1600 nm, with an active diameter of 0.10 mm and a rise time of less than 175 ps. The detector employs an FC input

connector to guarantee compatibility with fiber optic signals [188]. High-speed photodetectors can be utilized alongside any of the aforementioned monochromators, dependent upon the wavelength range.

2.2.3 Chemicals and equipment

- **Gases:** Helium (99.999%) as the driver gas, Argon (99.999%) as the driven gas, Nitrogen (99.999%), Oxygen (99.999%). These gases are supplied by Bhoruka Industrial Gases, India, and Chemix. Hydrogen gas is generated using a hydrogen gas generator by Chemlabs.

- **Chemicals:** The liquid and powder samples were purchased from the Tokyo Chemical Industry Co., Ltd. (TCI) and Sigma-Aldrich. The details are mentioned in individual chapters. Ethyl chloride (>99.7%) from Sigma Aldrich and 1,1,1-trifluoroethane (>99%) from Synquest Laboratories for calibration experiments.

- **Equipment:** The Edward (TCI pumping station) turbomolecular vacuum pump system, Adixen (ATP 400) turbomolecular vacuum pump, and the Agilent Vacuum Technologies (G8701A Turbo Pumping System) turbomolecular pumping system are used to evacuate the driven section up to 10^{-6} mbar before filling it up with argon gas. Depending on the required temperature (T5 and P5), the driven section is filled slowly with argon gas via a moisture trap cylinder (silica gel beads). The driver portion was emptied using the ED-30 rotary vacuum pump to a pressure of 10^{-3} mbar before being filled with helium gas. The bursting pressure on the driver section side varied from 30 to 90 bars depending on the diaphragm thickness and grooving.

2.2.4 Gas chromatography instrument

The quantification and identification of the pre-shock and post-shock gas mixtures were performed utilizing a gas chromatograph with a dual flame ionization detector (GC-FID/FID, Agilent 7890B) and a gas chromatograph coupled with a quadrupole mass detector (GC-MS, Agilent 7890A).

Figure 2.8: Gas chromatograph with a dual flame ionization detector (GC-FID/FID, Agilent 7890B) and a gas chromatograph coupled with a quadrupole mass detector (GC-MS, Agilent 7890A).

The flame ionization detectors of the gas chromatograph have been calibrated with hydrocarbons, utilizing known quantities of reference gases. The calibration procedure has yielded an estimated error of 5%. The mass spectrum of the mixture was then compared to the spectra from the NIST mass spectra database to ascertain which components had the closest spectral similarity.

The particulars of the gas chromatography are outlined below, taking into account the analysis duration and acceptable resolution for the hydrocarbon peaks in the analyses.

1. **Column details**: Light hydrocarbons ($< C_5$) have been measured using

gas chromatography with flame ionization detection (GC-FID) using HP-PlotQ columns. The high-mass hydrocarbons (C_5 and beyond) have been measured using the second flame ionization detector (FID) linked to the HP-5 column. In the gas chromatography-mass spectrometer (GC-MS) detector, we utilized a DB-1 column to specifically detect hydrocarbons with a mass-to-charge ratio (m/z) of > 42. The column length was 30 m for all three types.

2. **Split/splitless injection**: Splitless injection of our argon gas post-shock mixture samples at 200°C.

3. **Oven temperature ramp rate**: A temperature program (40 - 120°C) consists of the regulated heating of the oven at a consistent rate throughout the run for different time intervals.

4. **Carrier gas average flow rate**: Helium (He) and nitrogen (N_2) were used as carrier gases for gas chromatography-mass spectrometry (GC-MS) and gas chromatography-flame ionization detection (GC-FID) analyses. The carrier gas flow rate through the column in the GC-MS was kept at about 2 $cm^3min^{-1}$and in the GC-FID at about 30 cm^3min^{-1}.

2.3 Experimental procedure

The standard operating procedure (SOP) for executing an experiment in CST and MST is outlined as follows.

2.3.1 Start of a run

1. Installation of the grooved aluminum diaphragm at the diaphragm station.

2. Verify that the necessary gas cylinders for the experiment have sufficient pressure.

2.3.2 Sample loading in the CST facility

1. Evacuate the driven part via turbopump for two hours (pressure: approximately 10^{-5} mmHg).
2. Introduce the argon gas into the driven part to achieve a pressure of 500-600 mmHg (P1).
3. Close the pneumatically actuated ball valve.
4. Evacuate the test sample chamber (located below the ball valve, adjacent to the shock tube's end wall) using a turbopump for 45 minutes (pressure: approximately 10^{-5} mbar).
5. If the vapor pressure of the test sample is very low, the driven part is heated by a heating tube linked to a heater (maximum temperature of 120 °C).
6. Introduce the sample (2-3 mmHg) into the sample chamber via liquid nitrogen trapping through the freeze-pump-thaw methodology. Dilution of the sample by introducing Ar into the test sample chamber until a pressure of 500-600 mmHg (P1) is achieved. Permit this to mix uniformly for three hours.
7. Alternatively, if the vapor pressure of the test gas is high for the mixture preparation, a small mixing tank is utilized. This mixture can then be directly fed into the sample chamber.
8. Evacuation of the driver part via the rotary pump for 30 minutes (pressure: 10^{-2} mmHg).

9. For special cases such as the ignition delay measurement, the sample mixture includes oxygen in addition to argon.

10. The system is ready for the experiment.

2.3.3 Sample loading in the MST facility

1. Place the powdered sample on the sample holder plate before starting the turbopump.

2. Evacuate the driven part via turbopump for two hours (pressure: approximately 10^{-5} mbar).

3. Introduce argon gas into the driven part to achieve a pressure of 100-200 mmHg (P1).

4. In the event of adding a test gas, such as hydrogen, the closure of the pneumatically actuated ball valve is required. For example, argon gas is introduced into the driven portion at a pressure of 0.2 bar, while hydrogen is added at a pressure of 0.04 bar in the test section, resulting in a total gas mixture pressure of approximately 0.24 bar.

5. Evacuate the test sample chamber, situated next to the ball valve and adjacent to the shock tube's end wall, using a turbopump for 45 minutes (pressure: approximately 10^{-5} mbar).

6. Evacuation of the driver part via the rotary pump for 30 minutes (pressure: 10^{-2} mbar).

7. The system is ready for the experiment.

2.3.4 Performing the experiment

1. First, verify that all connections and signals are properly displayed in the DAQ display panel.

2. Then, the pressure in the driver section is gradually increased by introducing He gas from the control room. It is essential to monitor this pressure to accurately determine the diaphragm's rupturing pressure (P4).

3. The ball valve is designed to open prior to diaphragm rupture at a pressure closely aligned with the anticipated diaphragm rupture point. For instance, if diaphragm rupture occurs at approximately 10 bar, the ball valve is supposed to open when the rising driver section approaches approximately 8 bar.

4. The ongoing gas flow into the driver section will cause the diaphragm to rupture. Following diaphragm rupture, the ball valve must be rapidly closed, utilizing automated mechanisms with a manual override in the event of automation failure.

5. The post-shock mixture, intended for qualitative and quantitative analysis, is extracted from the end test section of the shock tube and subsequently transferred into a stainless steel cylindrical gas cell (Swagelok make). It is then promptly injected into GC-FID, GC-MS, FTIR, and other instruments to prevent condensation within the stainless steel cell.

6. In the case of collecting solid post-shock samples, the sample is collected by scraping off the surface of the test section after slowly venting the gases, so that small particles are not carried away.

2.3.5 Venting

1. Following sample analysis, the residual mixture in the test section must be evacuated from the shock tube via the gas line linked to the venting hood.

2. To ensure efficient venting of the post-shock mixture, the test section must be purged with argon gas and subsequently released to the external atmosphere through the hood.

3. The driven section must be evacuated by the turbopump for 30 minutes under heating conditions, provided the test section was heated during the experimental setup to eliminate any condensates.

2.4 Chemical Thermometry

The chemical thermometry method was developed based on Tsang's experiments [114] on the non-ideal temperature effects in shock tubes. In internal thermometry, the reflected shock temperature is determined by following the progress of an established reaction with a known rate constant, which is studied along with the reaction of interest. In external thermometry, experiments with the known reaction are done independently at different temperatures, and a calibration curve is plotted between the experimental and theoretical temperatures. According to Tsang's studies, the expression used for calculating temperature behind the reflected shock wave involving the use of an internal standard is

$$T = (\frac{E_a}{R})/ln(\frac{-1}{A*t}ln(1-((\chi))))$$

where t is the reaction dwell time, Ea is the activation energy, A is the pre-exponential factor for decomposition of the internal standard, and χ is the extent of the standard reaction.

$$\chi = \frac{[product]_t}{[product]_t} + [internalstandard]_t$$

where $[product]_t$ is the product concentration of the internal standard at time 't', and $[internal\ standard]_t$ is the unreacted concentration of the internal standard at time "t". The downside of the internal chemical thermometry methodology is that the internal thermometer may interact with other compounds in the test section during the reaction. In our experiments, we employ the external chemical thermometry method to calculate the temperature behind reflected shock waves. The obtained temperatures are then plotted against the reflected shock temperatures calculated using the conventional Rankine-Hugoniot method to obtain a linear correlation. Some of the chemical standards used are cyclopropane carbonitrile, ethyl chloride, 1,1,1-trifluoroethane, and cyclohexene [185].

The CST facility in our laboratory requires recalibration of the shock tube apparatus due to the incorporation of automation, the installation of pneumatic valves, and modifications to the shock tube's length to ensure precise measurements of the experimental reflected shock temperatures. The unimolecular decomposition of ethyl chloride (C_2H_5Cl) and 1,1,1-trifluoroethane ($C_2H_3F_3$) as the external standard was performed for the theoretical shock temperatures and pressures ranging from 950 to 1141 K and 8.3–12 bar for C_2H_5Cl and 1185 K to 1558 K and 12–24 bar for $C_2H_3F_3$ with a dwell time range from 1.32 to 1.60 ms. The concentrations of all the gaseous constituents of the experiment, including the reactant sample, pre-shock reactant sample, and post-

shock product mixtures, were estimated using gas chromatography with a dual flame ionization detector (GC-FID/FID). The gaseous components identified by GC-FID are ethyl chloride and ethene in C_2H_5Cl and 1,1,1-trifluoroethane and 1,1-difluoroethene in $C_2H_3F_3$. In the investigated temperature range, the HCl and HF elimination channel is the only thermal decomposition pathway.

$$C_2H_5Cl \rightarrow C_2H_4 + HCl$$

$$C_2H_3F_3 \rightarrow C_2H_2F_2 + HF$$

The pyrolysis of ethyl chloride and 1,1,1-trifluoroethane is weakly endothermic when present in very low concentrations. The effect of reactivity on the pressure trace is minimal, while the more significant changes stem from gas dynamic effects within the tube. Thus, to prepare the reactant mixture with argon gas, we take 1% of the reactants and let the mixing process occur overnight in a stainless steel gas cell. The sample gas showed only one GC peak in the FID.

The experimental temperature ($T_{5(kin)}$) for the given reaction has been calculated by putting the experimental rate constant values in the Arrhenius expression reported for thermal decomposition of ethyl chloride [189] for the temperature limit of 960 –1100K. From 2.1 it can be concluded that the rate of HCl elimination rises with the temperature within the experimental range.

$$k_{expt}(sec^{-1}) = 10^{13.84} \pm 0.20 \; exp\,[-\,(57.8 \pm 1.0\; kcal/mol)/RT]$$

$$T_{expt} = (57.8 \pm 1.0\; kcal/mol) \;/\; R \times [2.303 \times (13.84 \pm 0.20) - lnk_{expt}]$$

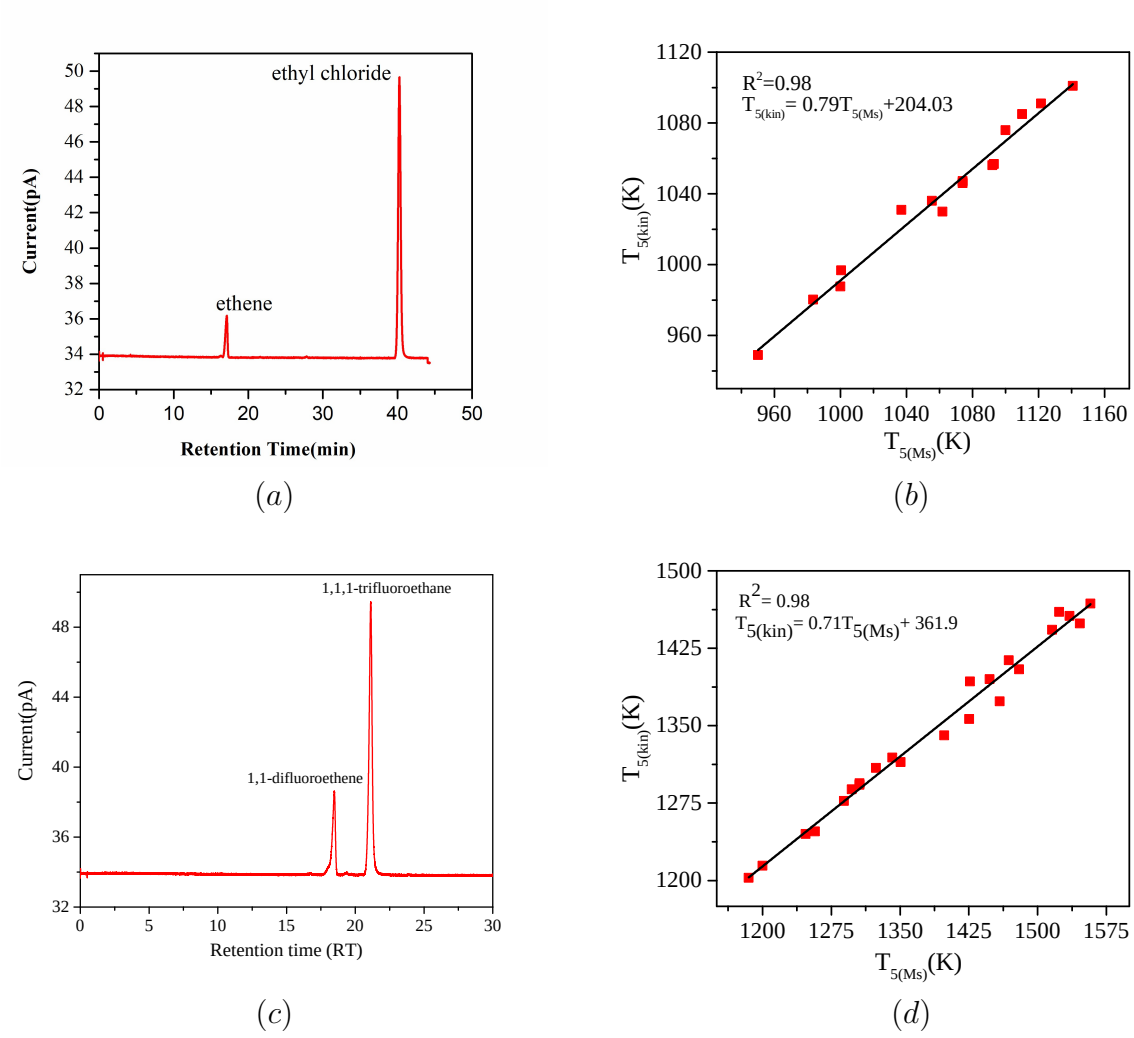


Figure 2.9: GC chromatogram for ethyl chloride and 1,1,1-trifluoroethane and temperature fits for chemical thermometry of the CST facility: (*a*) Chromatogram showing the separation of ethyl chloride and ethene in the GC column (HP-5 column), $T_{5(kin)}$ = 1036 K; (*b*) Plot of Experimental $T_{5(kin)}$ Vs theoretical $T_{5(Ms)}$ showing their correlation within the experimental temperature range 950–1141 K.; (*c*) Chromatogram showing the separation of 1,1- difluoroethene and 1,1,1- trifluoroethane in the GC column (HP-5 column), $T_{5(kin)}$ = 1288 K and (*d*) Plot of experimental $T_{5(kin)}$ vs theoretical $T_{5(Ms)}$ showing their correlation within the experimental temperature range 1185K -1558.

Table 2.1: Summary of the experimental results of ethyl chloride pyrolysis for Temperature calibration

S.N.	ms	$T_{5(Ms)}$(K)	$T_{5(kin)}$(K)	$[EC]_t/[EC]_0$	$[C_2H_4]_t/[EC]_0$	P5 (bar)
1	1.46	950	949	0.996	0.009	10.3
2	1.48	983	980	0.988	0.012	9.9
3	1.44	1000	988	0.986	0.014	10.1
4	1.42	1000	997	0.981	0.019	9.5
5	1.44	1037	1031	0.951	0.049	9.8
6	1.44	1055	1036	0.944	0.056	11.4
7	1.54	1062	1030	0.949	0.051	10.1
8	1.44	1074	1046	0.927	0.073	11.6
9	1.44	1074	1047	0.925	0.075	11.3
10	1.5	1092	1056	0.902	0.098	12.0
11	1.48	1093	1057	0.902	0.098	12.0
12	1.42	1100	1076	0.850	0.150	11.0
13	1.42	1110	1085	0.816	0.184	11.6
14	1.46	1122	1091	0.785	0.215	14.0
15	1.48	1141	1101	0.731	0.269	8.3

The experimental $T_{5(kin)}$ vs theoretical $T_{5(Ms)}$ is plotted in the figure. The least squares fitting method of this data has been performed to determine the experimental T_5 relation. This T_5 relation can be used as the actual experimental temperature for the upcoming experiments within the specified temperature range. The relationship between $T_{5(kin)}$ and $T_{5(Ms)}$ within the experimental temperature range of $T_{5\,(Ms)}$ of 950–1141 K is observed to be

$$T_{5(kin)} = 0.79T_{5(Ms)} + 204.03$$

The experimental temperature ($T_{5(kin)}$) for the reaction R2 has been calculated by putting the experimental rate constant values in the Arrhenius expression reported for the same reaction [190] for the temperature range of

1000-1600 K.

$$k_{exp}(sec^{-1}\ ) \ = \ 5.71 \times 10^{46} T^{-9.314} \exp(-47073K/T)$$

The experimental $T_{5(kin)}$ vs theoretical $T_{5(Ms)}$) is plotted in the figure. The least square fitting method of this data has been performed to determine the experimental T5 relation. The relationship between $T_{5(kin)}$ and $T_{5(Ms)}$ within the experimental temperature range of $T_{5\ (Ms)}$ of 1185K -1558K is observed to be:

$$T_{5(kin)} = \ 0.71 T_{5(Ms)} + \ 361.9$$

It can be clearly seen from the plot that the calculated temperature, $T_{5(Ms)}$ overestimates the actual temperature, $T_{5(kin)}$, and the difference increases with increasing temperature. The difference (between the two temperatures) observed at the higher temperatures is expected, as the T_5 calculation using conventional Rankine-Hugoniot relations does not account for the non-idealities in the reflected shock wave. Thus, for ethyl chloride and 1,1,1-trifluoroethane as external standard (T_{5kin}) were found to differ from $T_{5\ (Ms)}$.

Table 2.2: Summary of the experimental results of 1,1,1-trifluoroethane (TFE) pyrolysis for temperature calibration: DFE is 1,1-difluoroethene.

S.N.	ms	$T_{5(Ms)}$(K)	$T_{5(\mathrm{kin})}$(K)	$[TFE_T]/[TFE_0]$	$[DFE_T]/[TFE_0]$	P_5 (bar)
1	1.44	1185	1203	0.988	0.012	12.8
2	1.46	1200	1214	0.984	0.016	12.0
3	1.5	1247	1245	0.966	0.034	15.9
4	1.46	1257	1248	0.956	0.044	13.8
5	1.5	1289	1277	0.932	0.068	12.4
6	1.42	1297	1288	0.918	0.082	14.2
7	1.32	1306	1294	0.914	0.086	13.5
8	1.46	1306	1293	0.909	0.091	15.2
9	1.52	1324	1309	0.869	0.131	15.5
10	1.42	1342	1319	0.851	0.149	14.5
11	1.5	1351	1315	0.856	0.144	12.6
12	1.42	1398	1341	0.780	0.303	13.7
13	1.52	1426	1356	0.697	0.602	13.9
14	1.44	1426	1393	0.509	0.491	18.9
15	1.58	1448	1395	0.463	0.799	16.3
16	1.6	1459	1374	0.591	0.220	15.5
17	1.36	1469	1413	0.398	0.537	16.2
18	1.54	1480	1405	0.409	0.591	13.8
19	1.42	1516	1443	0.201	0.889	17.0
20	1.4	1524	1460	0.120	0.880	18.6
21	1.48	1535	1456	0.123	0.877	24.1
22	1.52	1546	1449	0.149	0.851	15.5
23	1.52	1558	1468	0.073	0.927	22.7

2.5 Computational methods

2.5.1 Quantum chemistry calculations

Ab initio methods were employed to determine all the stationary points, including the ground state, transition state, and products. These results were then utilized in the transition state theory (TST) calculation to ascertain the kinetics of the unimolecular decomposition processes. CASSCF/MRCI (multireference) [191, 192] , and CBS-QB3 (single reference) [193] approaches have been utilized for the computations. The stationary points were confirmed using a harmonic vibrational analysis and were classified as either a minimum or a transition state based on the presence of one imaginary frequency along the reaction coordinate. The number of imaginary frequencies dictates the nature of the stationary point in the geometry: 0 for a structure that is a local or global minimum in the potential energy hypersurface and 1 for a transition state. According to the standard transition state theory, the saddle point in a reaction is considered the bottleneck since it has the most electronic energy. Intrinsic Reaction Coordinate (IRC) calculations are performed in both directions (reactant and product), beginning with the optimized transition state structure, and the saddle point is confirmed.

The multireference configuration interaction (MRCI) method integrates the multiconfiguration self-consistent field (MCSCF) approach, with the complete active space self-consistent field (CASSCF) being the most commonly utilized method, alongside traditional configuration interaction (CI) techniques. The geometry optimizations and frequency calculations were performed utilizing the CASSCF (complete active space self-consistent field) (zero-point energy (ZPE) scaling factor is 0.932) method with the 6-31+g(d,p) basis set. Correc-

tions to single-point energies have been performed using the MRCI approach with a similar active space and basis set. The unstable biradical intermediates participating in the ring-opening isomerization and unimolecular decomposition reactions (e.g., extended C-C and C-H bond lengths during bond dissociation) involve multireference calculations. The CBS-QB3 method was employed to compute the H-abstraction and subsequent radical decomposition processes, among others. In the first step, the geometry optimization and frequency calculations were conducted using the B3LYP (Becke 3-parameter Lee-Yang-Parr) [194, 195] hybrid density functional method with the 6–311G(2d,d,p) basis set (zero-point energy (ZPE) scaling factor of 0.99). The second step involves complete basis set extrapolation to correct the total energy. Multireference computations were conducted using the Molpro 18 and 24 quantum chemistry software [196]. The remaining single reference computations were conducted using the Gaussian 16 program [197].

2.5.2 Reaction rate constant calculations

High-pressure limit thermal rate constants for all the elementary reactions associated with a saddle point (transition state) were calculated utilizing conventional transition state theory (TST).

$$k(T) = \sigma \frac{k_B T}{h} \frac{Q_{\neq}}{\Pi Q_R} exp(-\frac{\Delta E_0}{RT})$$

where σ is the symmetry number, k_B is the Boltzmann constant, h is the Planck's constant, T is the temperature, Q_R is the total molar partition function for reactants (consisting of the translation, vibration, and rotation), $Q_{\neq}$ is the partition function of the activated complex, and ΔE_0 is the electronic energy barrier, including ZPE. To compute the activation energy barrier (ΔE_0),

the reaction path has been defined as the path with a minimum energy along the potential energy surface that links the reactants and products while traversing the transition state. The C-H bond dissociation channel is a barrierless reaction requiring a variational treatment. The position of the transition state relative to the temperature was determined using a variational method, which minimized the rate constant as a function of the reaction coordinate(s) and temperature (T) within the specified temperature range (800-2000K).

$$k_{VTST} = min k_{TST}(s, T)$$

where $k_{TST}(s, T)$ represents the rate constant at each location along the reaction coordinate. To implement chemical kinetic modeling effectively, three kinetic parameters, A, n, and, E_A are determined by fitting the calculated rate constants across a temperature range of 800-2000 K in increments of 50 K to a modified Arrhenius equation. The kinetic parameters A, n, and, E_A are ascertained by fitting the computed rate constants throughout a temperature range of 800-2000 K in 50 K intervals to a modified Arrhenius equation. Considering the reasonable correlation obtained with the temperature coefficient, which yielded a value of n = 0 within the studied temperature range, we decided to maintain the temperature coefficient at zero. The modified Arrhenius equation for n=0 is shown below.

$$k(T) = Aexp(-\frac{\Delta E_a}{RT})$$

The calculations of the rate constants were performed utilizing the Multiwell 2023 program package [198, 199, 200]. The thermal module of the multiwell allowed conventional transition-state theory (TST) calculations, while the ktools module was employed for variational transition-state theory (VTST) cal-

culations. Partition functions were calculated using the vibrational frequencies and rotational constants obtained from the quantum chemistry calculations mentioned in the previous section. In most cases, internal degrees of freedom were regarded as rigid rotor harmonic oscillators. It is important to emphasize that the limited rotations of the cyclic structure were also considered harmonic oscillators, which included flexible movements of the ring. On the other hand, the unrestricted alkyl groups (e.g., internal rotation of the methyl group) were viewed as one-dimensional hindered internal rotors. The internal rotors were considered using the hindered rotor feature of the Gaussian 16 program, with hindrance potentials calculated at the B3LYP/6-311G(2d, d, p) level. The potential energy for each internal rotation of the reactant was calculated by performing a relaxed energy scan of the dihedral angle at 10-degree intervals (36 steps for 360 degrees). For the transition state, the potentials of hindered internal rotations, which are nearest to the reaction sites, were calculated with the bond lengths at the critical geometries held constant (using the bond freeze option in Gaussian 16). This study excluded the quantum tunneling effect because of the comparatively low barriers associated with reactions involving H atoms, such as H-abstraction and H-migration, and the high temperatures investigated.

2.5.3 Chemical kinetic modelling

The primary factor in accurately reproducing combustion characteristics under defined conditions is the verification of each species in the shock tube analysis. Validations were performed using CHEMKIN-PRO software [201]. The shock tube simulation required the identification of the products, based on the assumptions of homogeneity, adiabatic conditions, and constant volume.

Chemical kinetic models for hydrocarbons have been developed by integrating previously established base mechanisms into existing frameworks. To reduce inaccuracies resulting from the omission of isomers and less significant reaction pathways, the rate parameters for specific reactions within the sub-mechanisms are modified. The iterative process of steps (1) and (2) continues until the mechanism can consistently replicate the primary species evolutions across a wide range of operating temperature and pressure conditions.

1. The purpose of conducting sensitivity analysis is to identify the critical reactions that significantly influence the pyrolysis studies. The reaction rates of these processes are adjusted to achieve a satisfactory correlation with the speciation data for the combustion studies.

2. Further refinement is accomplished by integrating route analysis with production rate (ROP) analysis results to accurately replicate the changes in the concentrations of key species.

The generation of thermochemical data employs the Reaction Mechanism Generator (RMG) [202], which integrates the Benson group additivity method and, when required, quantum mechanical calculations to predict properties such as enthalpy of formation, entropy, and heat capacity.

Chapter 3

Shock processing of coronene

Part of this chapter is published in a journal

Title: Shock-induced evolution: tracing the fate of coronene in astrophysical environments.

Authors**: D.K. Singh**, L. Biennier, A. Simon, S. Chakraborty, E. Dartois, R. Georges, S. Kassi, V. Chandrasekaran, H. Sabbah, C. Joblin, S. Ranjan, S. Suwas, G. Jagadeesh, and E. Arunan. *Accepted: Astronomy & Astrophysics (A&A) journal.* [203]

Abstract of the chapter

Context: Polycyclic Aromatic Hydrocarbons (PAHs) are considered ubiquitous in the interstellar medium. Evidence for their presence in the literature is abundant; however, the mechanisms of formation and evolution continue to be a topic of debate. The shock processing of PAHs remains an underexplored aspect among the various processes influencing their evolution in the interstellar medium. The objective of this study is to investigate the shock processing of coronene ($C_{24}H_{12}$), a representative pericondensed PAH, and to analyze the gaseous volatiles and solid residues through both in situ and ex situ techniques.

Experimental and computational methods: The MST facility was employed to sublimate and heat coronene and related analogues to temperatures of 4000 K, which are somewhat similar to conditions encountered during low-velocity shocks in the ISM. The primary focus of the study was the time evolution of shock products in situ, analyzed through optical emission spectroscopy on a microsecond timescale. This study is further supported by other components such as corannulene ($C_{20}H_{10}$), fullerene (C_{60}), fullerene (C_{60}) with hydrogen and ethylene (C_2H_4). The results were supported by the collection and analysis of solid residues post-shock, as well as by molecular dynamics (MD) simulations.

Results and conclusion: In situ spectroscopy confirmed the presence of C_2 radicals, a broad continuum emission, and a broad green component, which is attributed to smaller C_nH_x hydrocarbons. Ex-situ analysis of solid residues demonstrates the formation of graphitic and graphenic nanostructures. MD simulations reveal that dehydrogenation and fragmentation processes occur during shock processing, which are essential for the formation of C_nH_x and smaller CH, C_2, C_3, etc. fragments important for emission studies.

The identification of C_nH_x species as potential carriers of a broad green emission observed in the laboratory is an important finding, indicating a possible connection to the 5450 diffuse interstellar band (DIB). This DIB carrier was not only found in coronene but also in smaller hydrocarbons. Shock processing may serve as a mechanism to connect the top-down and bottom-up pathways in the interstellar medium (ISM), as demonstrated by the extensive green emission feature attributed to the C_nH_x species, which is correlated with the λ5450 DIB feature observed in both experiments. Finally, shock waves promote the transformation of polycyclic aromatic hydrocarbons (PAHs) into both smaller

and larger hydrocarbon clusters during the hot phase, and into graphitic nanostructures upon cooling, thus affecting the destruction and evolution of carbon analogs in the interstellar medium.

3.1 Background

Shock waves are ubiquitous in space, driven by events such as supernova explosions, outflows from forming stars, cloud-cloud collisions, or stellar winds. Their propagation leads to a sudden compression, heating, and particle acceleration. They are considered to actively participate in the physical and chemical evolution of the interstellar medium. Shocks can increase the PAH abundance by breaking down large grains through collisions with fast atoms or ions, but also decrease it by destroying them directly. The effect of shock waves on carbon dust analogs or building blocks can complementarily be explored with the help of shock tubes [115, 3], and analogous studies on, e.g., amorphous carbon nanodust [117].

Earlier investigations concentrated mostly on fullerene, specifically C_{60}. The authors [115, 3] performed ex-situ and in-situ chemical investigations to attain an in-depth understanding of the chemical evolution of C_{60} fullerene under shock wave environments. In the first study, the authors investigated the thermal processing of fullerene C_{60} in hydrogen throughout a gas temperature range of 783 to 4271 K by means of ex-situ investigation of the post-shocked samples. The ex-situ analysis of solid residues utilizing techniques that characterize physical (transmission electron microscopy, scanning electron microscopy, X-ray diffraction) and chemical structures (infrared spectroscopy, Raman spectroscopy, laser desorption laser ionization mass spectrometry) was conducted and revealed the conversion of C_{60} into an amorphous material. The

chemical analysis of the post-shock gases was performed using gas chromatography and cavity ringdown spectroscopy. In the second study, the authors concentrated on examining the shock-induced processing of C_{60} at high temperatures ($\leq$4500 K) by optical emission spectroscopy and molecular dynamics investigations.

A hypothesis states that the 3.3 μm PAH emission band, commonly detected in UV-intense reflection nebulae, planetary nebulae, and HII regions[6], primarily arises from small PAHs comprising 20–30 carbon atoms [204]. Under intense UV radiation, compact, pericondensed PAH molecules, such as coronene and ovalene, exhibit a higher likelihood of survival compared to catacondensed PAHs characterized by an open, irregular structure. Coronene, characterized by its symmetric and stable structure, has been used as a prototypical PAH in various experimental and computational studies, as outlined in the introduction section previously. Therefore, in the current work, we investigate the stability of coronene ($C_{24}H_{12}$), a PAH, against shocks by combining laboratory experiments and theoretical calculations similar to fullerene studies. One of the long-term goals that is being pursued is to contribute to a better understanding of the life cycle of carbon in space.

The analysis of coronene's shock-induced emission components has been further supported by the complementary experiments on corannulene ($C_{20}H_{10}$), fullerene (C_{60}), fullerene (C_{60}) with hydrogen and ethylene (C_2H_4). The experiment samples are displayed in the comparison section 3.4.9. These selections are aimed at improving our understanding of the findings presented in the current investigations. Corannulene is a PAH distinguished by its distinctive bowl-shaped structure. Unlike the flat, planar structure of traditional PAHs like coronene, corannulene's curvature is a defining characteristic, earning it

the title of "buckybowl," as it can be thought of as a portion of the larger fullerene, C_{60}. Ethylene has been chosen as the smaller hydrocarbon component. Relevant comparisons from the previous two studies on fullerene are also made for the experiments.

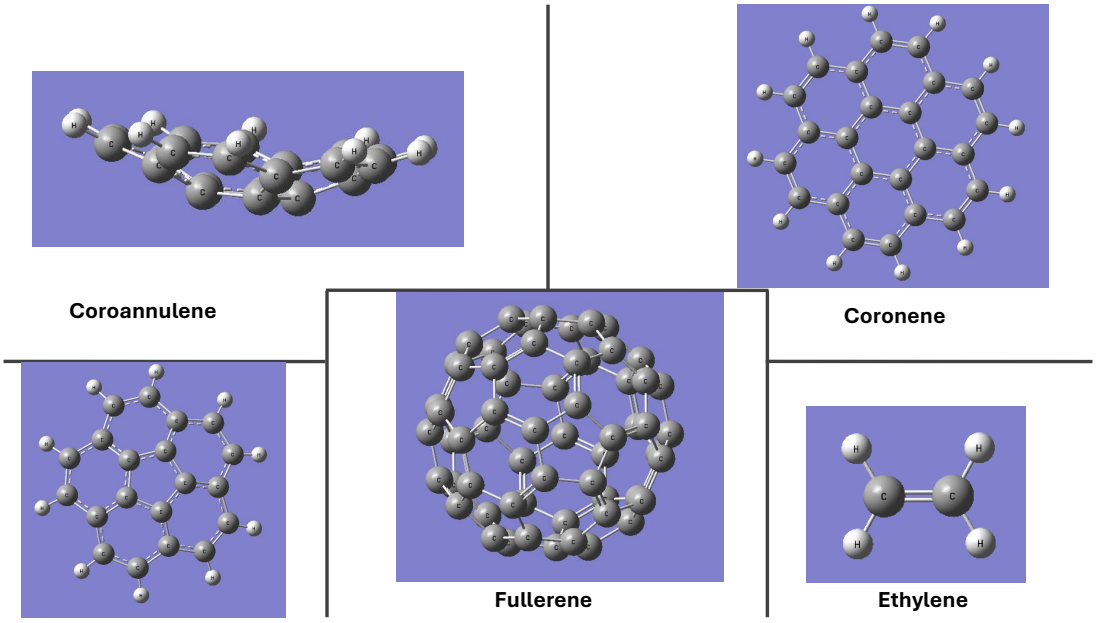


Figure 3.1: PAHs (coronene and coroannulene), fullerenes, and hydrocarbons are studied in this chapter.

This chapter is organized as follows: the experimental methodology to study the *in situ* chemical evolution of coronene is described in section 3.2 while the associated emission spectroscopy results follow in section C and 3.4. IVR studies are briefly discussed in the section 3.5. The major part of this chapter is focused on the *in situ* emission spectroscopy studies and analysis.

The findings from the emission spectroscopy studies are supported by further modeling and ex-situ analysis carried out by our collaborators, summarized concisely. Molecular dynamics (MD) simulations (section 3.6) were carried out to help in the understanding of the destruction processes. *Ex-situ* analyses of the solid residues were conducted (section 3.7) in parallel using laser desorption laser-ionization mass spectrometry (L2MS), X-ray diffraction (XRD), micro-Fourier transform infrared spectroscopy (μ-FTIR), Raman spectroscopy,

and infrared spectroscopy to get some insight into the chemical structure of the shock products. Scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (HRTEM) were finally employed to shed some light on the physical transformations of the sample.

This chapter includes a detailed discussion based on all the findings in section 3.8 , and also the astrophysical implications of the work are mentioned in the section 3.9. The section 3.10 contains the summary of the work done in this chapter.

3.2 Experimental setup

The detailed description of the experimental setup can be found in Chapter 02 in Sec.2.1. Here, a brief description relevant to the experiments discussed in this chapter is given.

3.2.1 Material Shock Tube facility

For this study, we employed the Material Shock Tube (MST) facility, designed to study how shockwaves interact with solids and gases in ways that are relevant to astrophysical conditions. It is equipped with a sample chamber (Fig. 3.2), which is the centerpiece of the facility. About ∼2-3 ms of dwell time was achieved with the 2.1 m long driver section. The sample chamber consists of part of the driven section after the ball valve, the sample holder, the extension part, the optical chamber, and the end flange. The sample chamber, the optical flange with lens holders, and the end flange have been made from aluminum to avoid surface contamination that can show up in the case of stainless steel.

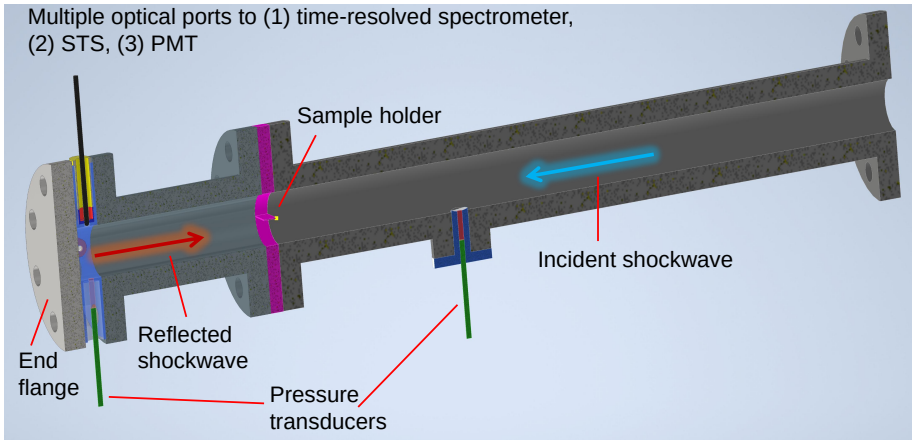


Figure 3.2: Schematic representation of the sample chamber of the Material Shock Tube facility used to study the *in situ* chemical evolution of interstellar dust analogues.

The experiment used an aluminum diaphragm of 1-2 mm thickness and variable grooving for bursting.

3.2.2 Chemicals and gases

The experiments performed in the MST facility focused on *in situ* and *ex situ* analyses of the powdered sample and gaseous samples. The coronene $C_{24}H_{12}$, (mol. wt. = 300.36 u), corannulene ($C_{20}H_{10}$), (mol.wt. = 250.29 u), fullerene (C_{60}) (mol. wt. = 720.66 u) powder were purchased from the Tokyo Chemical Industry Co. Ltd., with >98% purity, and ethylene (C_2H_4) (mol. wt.=28.05 u) gas from Bhoruka gases. The stainless-steel-built sample holder placed in the sample chamber is loaded with 6 to 30 mg of sample, ready for shock wave exposure. Ultra-high-purity helium (99.999%) as the driver gas and argon (99.9999%) as the driven gas are used for all the experiments with the MST. A hydrogen generator has been utilized for the runs that require hydrogen. A small turbomolecular pump is used to evacuate the driven section down to 10^{-6} mbar before filling it up with argon. Depending on the required temperature (T_5), the driven section is filled slowly with 0.14-0.47 bar of argon via a moisture trap cylinder (silica gel beads) to avoid sample disruption. The

driver portion is emptied using a rotary vacuum pump down to a pressure of 10^{-3} mbar before being filled with helium. The bursting pressure on the driver section side varied from 50 to 90 bar depending on the diaphragm thickness and grooving.

3.2.3 Data Acquisition System (DAQ)

The data acquisition is handled by a National Instruments System (USB-6356 DAQ card) and a Digital Storage Oscilloscope (Tektronix model TBS 2000B series). It reads the output of 3 PCB pressure transducers (PT1, PT2, and PT3 sensors model 113B24 with 5 mV/psi) through PCB signal conditioners with amplification (model 441A42) as well as static pressure gauges and indicators. The NI-DAQ and the Tek oscilloscope are triggered by the PCB sensor mounted in the shock tube's driven section to obtain the pressure profiles and the monochromator PMT signal. The NI-DAQ card triggers the STS spectrometers and the NECTA Line Scan Camera (high-speed CMOS camera) by sending a 5 V TTL pulse. The time intervals between the rising fronts of the pressure trace from the incident shock are utilized to calculate the incident shock velocity and Mach number. The temperature and pressure behind the reflected shock waves were calculated from the Mach number using the standard one-dimensional normal shock equations from the Wisconsin Gas Dynamics Calculator [1]

[1] https://silver.neep.wisc.edu/~shock/tools/gdcalc.html

3.3 Emission spectra analysis

3.3.1 Introduction (C_2)

The C_2 radical is the simplest carbon cluster, but its electronic spectrum is very rich and complex. C_2 is detected in various astronomical entities, such as stars, circumstellar shells, nebulae, comets, and the interstellar medium. C_2 is also responsible for the green-blue glow associated with hydrocarbon flames. C_2 plays a crucial role in astrochemistry and combustion research, as shown in Figures 3.3 and 3.4. Optical spectroscopy enables the observation of absorption and emission phenomena across the infrared, visible, and ultraviolet regions of the spectrum. Being a homonuclear diatomic molecule, it does not possess a permanent electric dipole; thus, the absence of electric-dipole-allowed vibrational or rotational transitions renders its spectral emission signature a sensitive indicator of the local surroundings. As a result, it is not readily detectable via its rotational or vibrational spectrum and is solely disclosed through its extensive electronic spectroscopy. This molecule possesses eight valence electrons distributed across 16 valence spin-orbitals, demonstrating a wider range of valence electronic configurations and electronic states compared to any other second-row homonuclear diatomic molecule [2].

Among the 19 documented electronic bands 3.5, this discussion centers on the Swan Band. Figure 3.6 illustrates the ground ($a_3\Pi_u$) and excited state ($d_3\Pi_g$) electronic energy levels of C_2 within the Swan system, accompanied by an example of vibrational transitions.

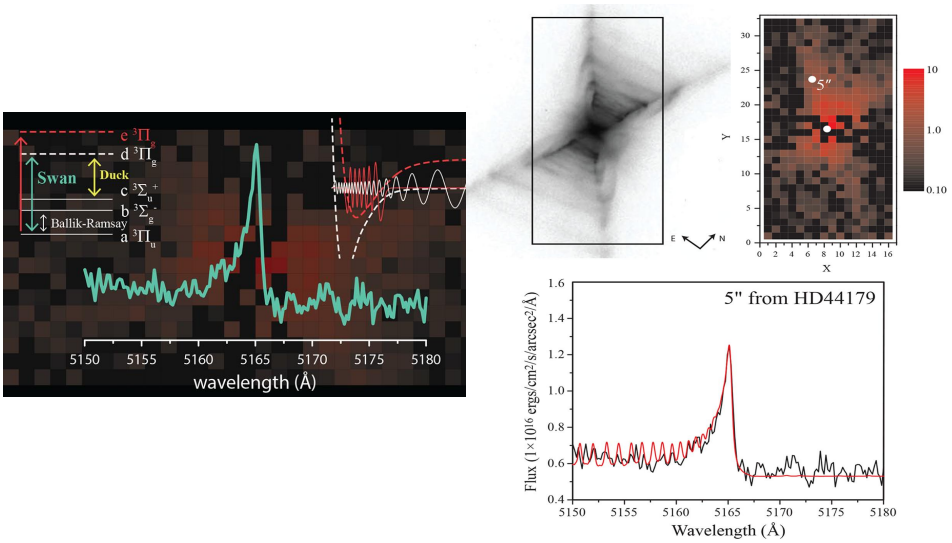


Figure 3.3: *C_2 in astrochemistry*: On the *left side* the image shows the 516 nm Swan band peak. On the *right side* ((top left) Hubble image of the Red Rectangle (HD 44179) depicting the area analyzed by SPIRAL (NASA; ESA; Hans Van Winckel, Catholic University of Leuven, Belgium; Martin Cohen, University of California, Berkeley). (top right) The integrated (0–0) Swan band intensity map in the Red Rectangle (HD 44179) distinctly outlines the nebula's shape (Robert Sharp, AAO; Damian Kokkin, University of Sydney). (bottom) Representative Swan band spectrum obtained 5 arcseconds from the central object. (Adapted from [2] with permission).

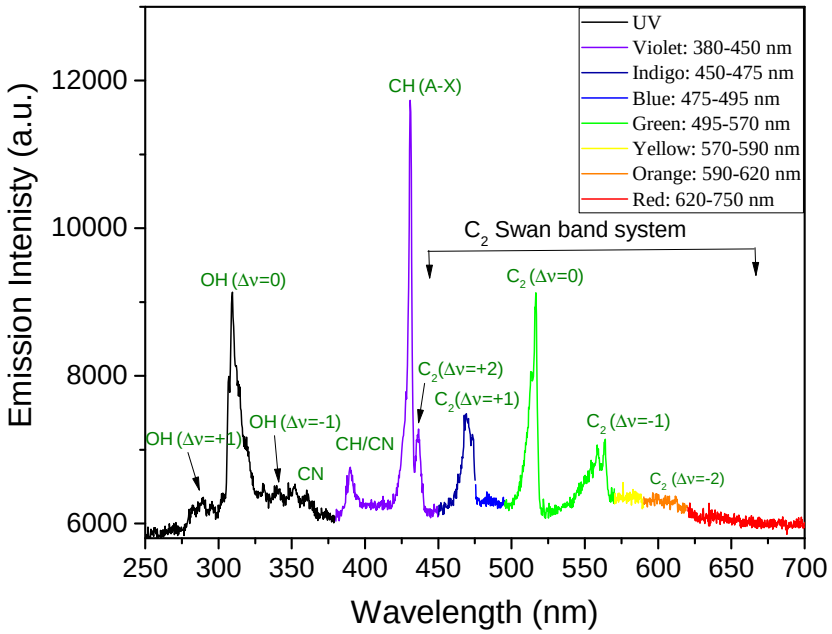


Figure 3.4: *C_2 in combustion*: Flame emission spectra taken from a butane lighter flame showing different species, including C_2 species dominating in the visible region.

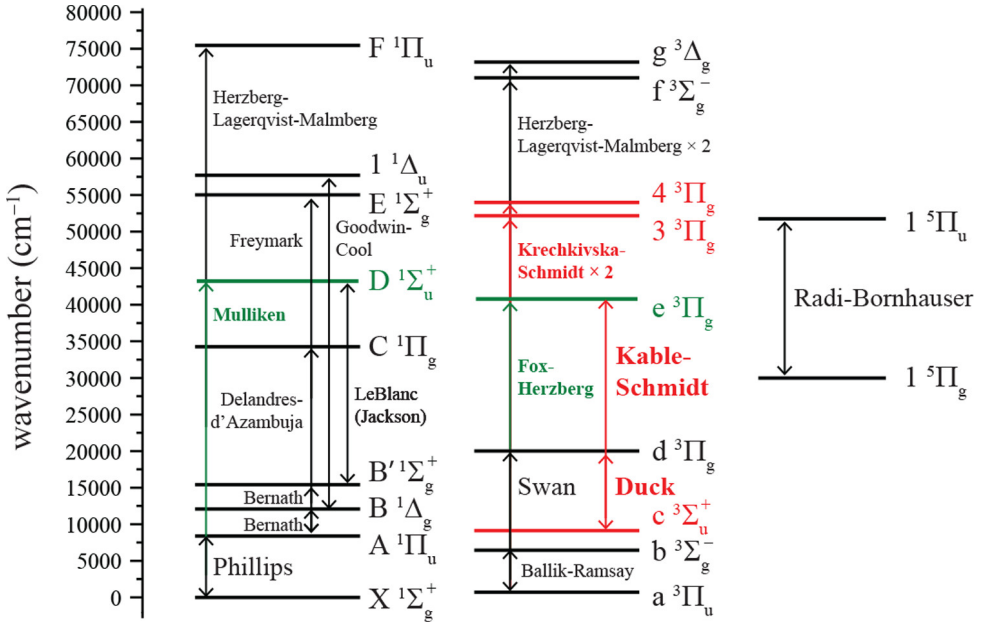


Figure 3.5: C_2 bands [2] (Adapted from [2]) with permission

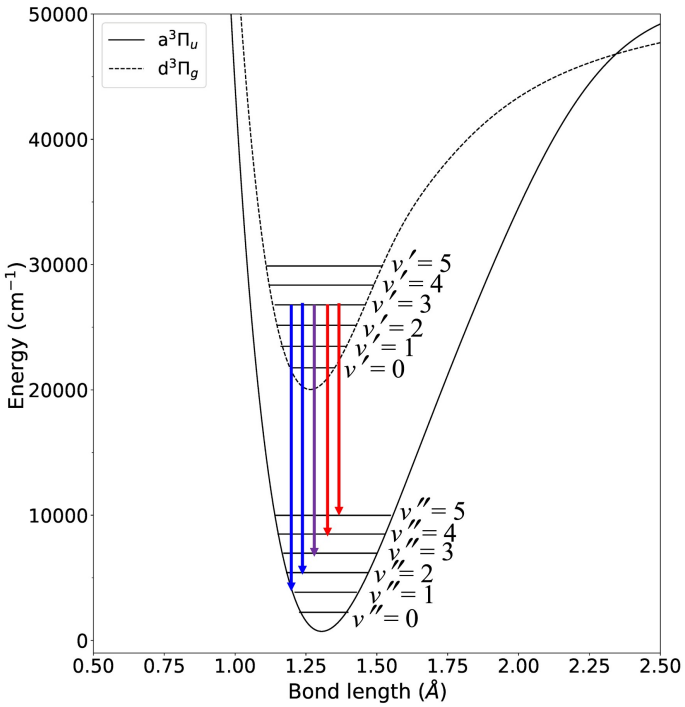


Figure 3.6: Ground ($a^3\Pi_u$) and excited ($d^3\Pi_g$) electronic states of the Swan system C_2^{12}. The $\Delta v = +1$ and $+2$ transitions are in blue, the $\Delta v = 0$ transition is in purple, and the Δv = -1 and -2 transitions are in red [3].

3.3.2 Time-resolved emission spectroscopy

The following sections describe the development of a time-resolved broadband emission spectrometer for studying the C_2 Swan band.

Initial studies

The fullerene C_{60} was discovered 37 yr. ago in the laboratory by Kroto et al. [26] during experiments aimed at understanding the formation of the longer-chain carbon molecules in the interstellar space and circumstellar shells of late-type stars. Biennier et al. [115] studied the impact of a shock wave on crystalline particles of C_{60} in the presence of hydrogen in a shock tube at temperatures around 4000 K. The study showed the formation of smaller hydrocarbons such as CH_4, C_2H_6, C_2H_4, and C_2H_2 on shock processing of C_{60}. The experiments that were conducted in 2019 by Chakraborty et al. [3] were aimed at observing the different transitions of the molecules via a fast spectrometer by integrating over the whole duration of the experiment. In addition, the spectral and temporal measurements were performed on a single wavelength from a monochromator. Following these results and questions raised from the literature and our own studies, the aim is to develop tools for emission measurements over the broadband spectrum with time resolution during the shock process along with the methods used earlier. This present work will demonstrate the tool developed for emissions of *C_2 swan band* with time during the shock processing. Such experimental measurements are often complicated in the shock tubes because of a lack of accurate methods. Directly detecting many radical species due to their short lives and low steady-state concentrations is challenging. To deal with these open questions, the experimental detection method must have certain characteristics, such as high

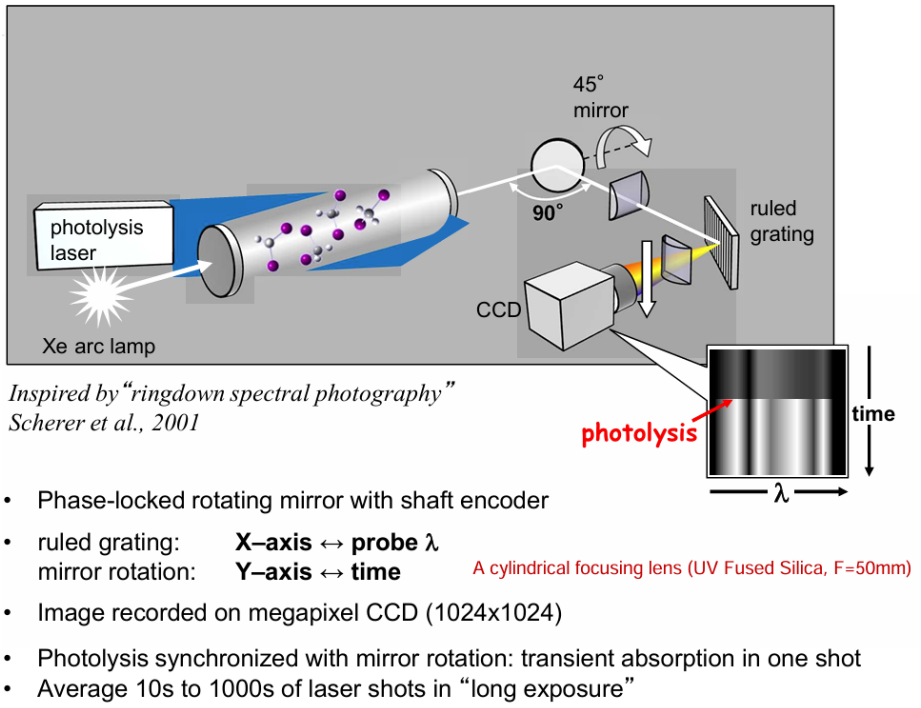


Figure 3.7: TR-BB-CEAS (time-resolved broadband cavity enhanced absorption spectroscopy) experimental setup. The TR-BB-CEAS configuration comprises a white-light probe source, a broadband optical cavity incorporated with a photolytic-initiation chemical reactor, and a time-resolved spectrometer.

sensitivity for detecting lower concentration species, multiple species detection at the same reaction time, and time-resolved measurements.

The initial experimental setup is based on a presentation by Leonid Sheps, who outlines the configuration of a fast absorption spectrometer designed for diagnosing photolysis processes via laser (see figure below 3.7). The initial assembly adopts the concept of the Sheps spectrometer [205], specifically tailored to address our objective of conducting rapid emission spectroscopy of electric arcs.

The final spectrometer must attain both spectral and temporal resolution. A diffraction grating facilitates the horizontal dispersion of the incident beam by wavelength, allowing for the acquisition of the spectrum of the electric arc. A galvanometric mirror will conduct a vertical scan of the complete output spectrum on the CMOS camera. Figure 3.8 demonstrates the principle

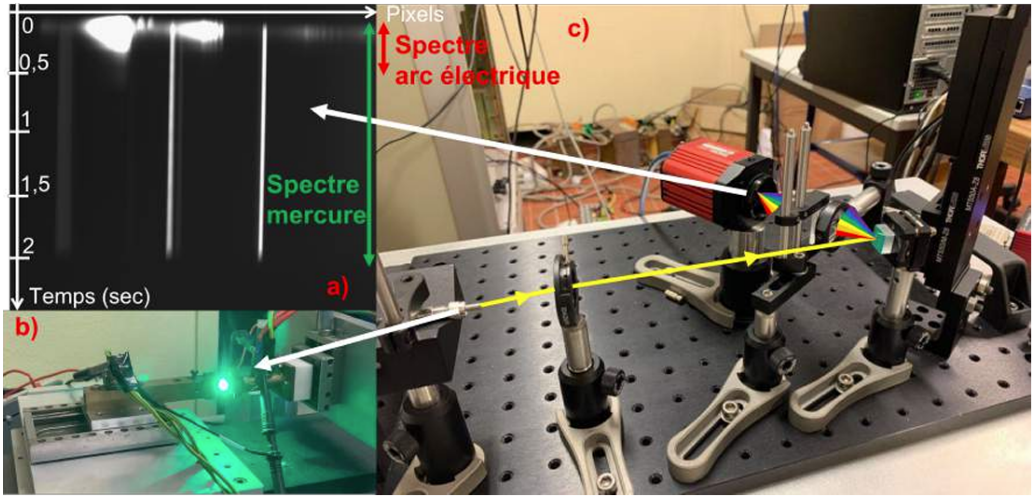
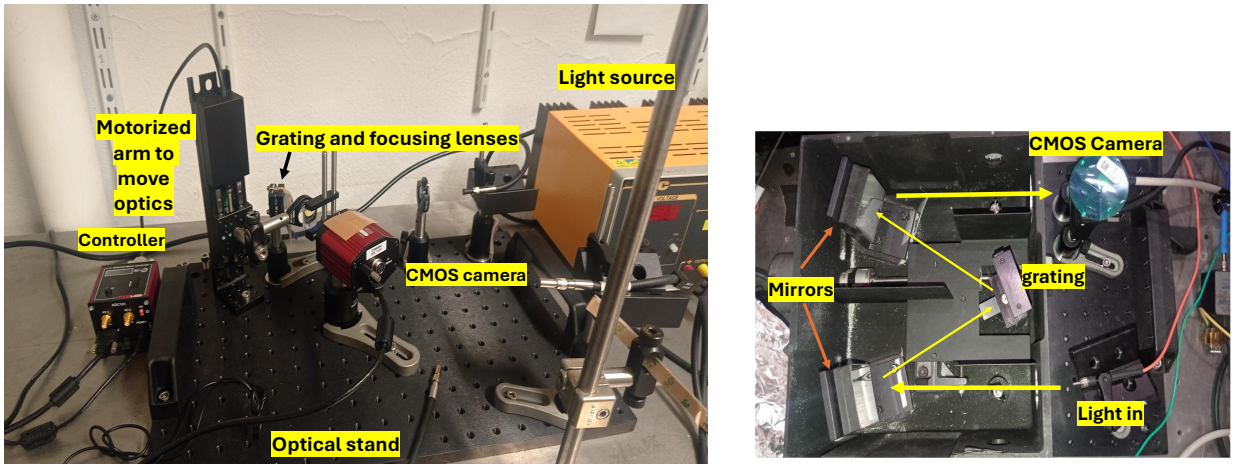


Figure 3.8: Initial studies for the development of a fast spectrometer for the diagnosis of electric arcs (Image from "Development of a fast spectrometer for the diagnosis of electric arcs by Lorenn Turnier"). The figure shows the summary of the final assembly of the initial spectrometer setup: a) spectrum obtained from CMOS camera b) photo of electric arc c) final assembly of the time-resolved spectrometer

underlying the acquisition of time measurements. Finally, spectral and temporal information will be acquired from the CMOS camera and subsequently retrieved directly on the computer.

The figure 3.9 shown below was assembled on the same principle intended for attachment to the shock tubes. Unfortunately, the final setup could not be applied in the MST facility for certain reasons. The galvanometric mirror equipped with a motorized arm exhibited insufficient speed to record the shock event within 10 ms. The response time for the entire scan associated with a single trigger event was insufficient to adjust the mirror by a few degrees. The old mono setup with a stepper motor configuration experienced similar issues and inadequate resolution. Moreover, the earlier setups discussed in Fig. 3.7 and 3.8 were meant for continuous acquisition of the spectra with integration time in seconds.



(a) (b)

Figure 3.9: Initial assembly of the spectrometers (*a*) Setup was done in Rennes, France. This includes the cables, light sources, optical cable, mirrors, lenses, stand, nuts, and optical table with (18*12) (25 mm) between each holes. (*b*) Old monochromator setup with a CMOS camera (gratings are moved with a stepper motor).

Time-resolved spectrometer

The final setup shown in figure 3.10 includes a manual monochromator and a high-speed CMOS camera. The refurbished monochromator was utilized to collect a small wavelength window of light from the emission in the shock tube and supply it to the camera. One of the optical ports is connected through a 1000 μm optical fiber to a new home-built time-resolved spectrometer, which includes a refurbished manual monochromator and a high-speed camera.

It is composed of a Newport 77298 grating assembly, ruled with 1200 grooves/mm, 360 nm blaze, to operate in the 200-1000 nm wavelength region. The opening slit can be finely adjusted with a width that can vary from 4 μm to 3 mm and a height that can be adjusted between 2 and 12 mm. The design is derived from the Ebert-Fastie concept, employing a single large spherical mirror to collimate point light entering the input port and to concentrate the diffracted light from the grating at the output port. A resolution of up to 0.1 nm is achieved with the current grating. The central wavelength is chosen by manipulating a manual wavelength selector on top of the monochromator.

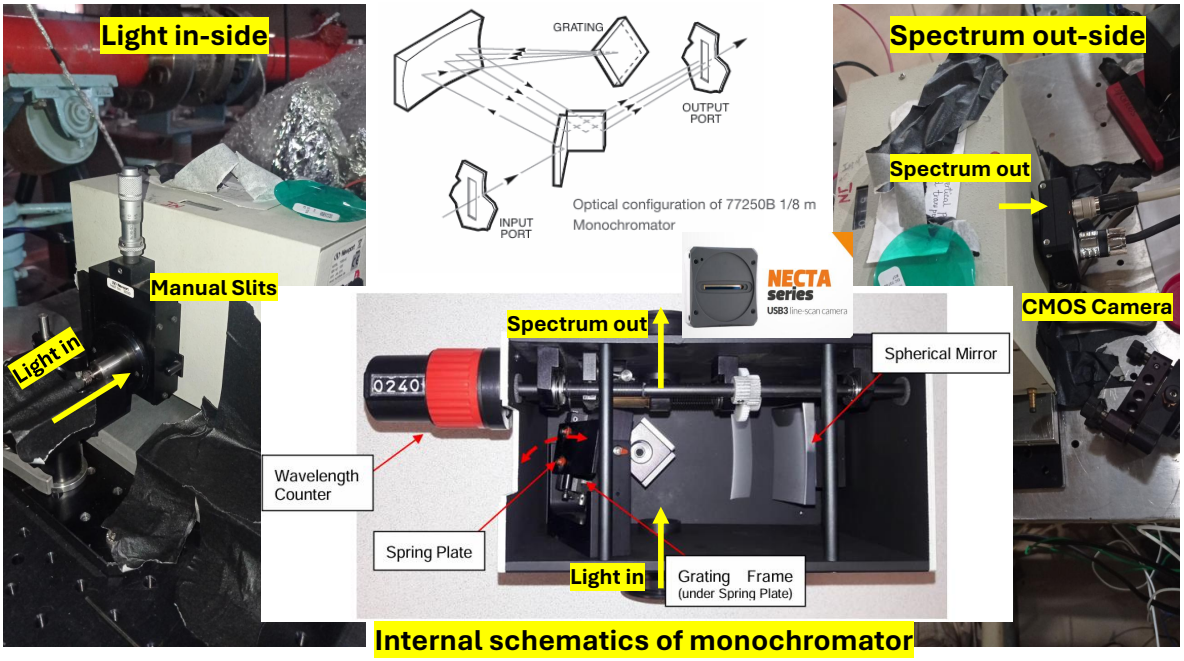


Figure 3.10: Home-built spectrometer setup: manual monochromator with a high-speed CMOS camera. On the light inside, the slits are attached to the optical fiber along with the collimator. On the spectrum outside, a high-speed CMOS camera is attached to capture the spectrum.

The exit slit is removed and replaced by a line scan monochrome camera (Sensor type Mono Sensor resolution 1(H) x 4096(W) with a pixel size 3.5 μm $\times$ 3.5 μm – Alkeria Necta N4K-7). The maximum time resolution that can be attained is 10.6 μs.

The camera operates under the frame acquisition mode; the transient wavelength-resolved emission measurements are collected onto the array of CMOS sensors. A 42.3 μs resolution has been selected to acquire the timed data from the CMOS line camera for the mentioned experiments. The choice of the camera's frame rate was based on factors such as the readout intensity, readout noise, and dark noise during very short integration times. The recording sequence comprises a matrix of time and wavelength data, as shown in Fig. 3.11

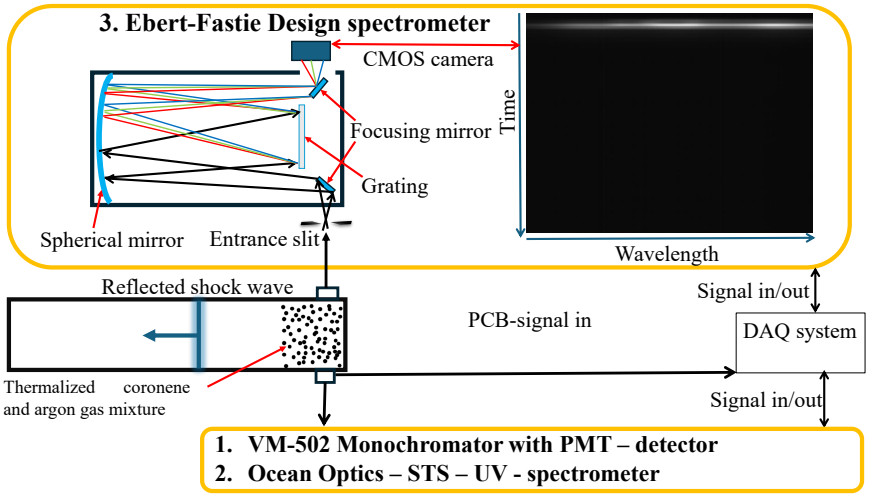


Figure 3.11: Optical setup showing the raw image obtained from the CMOS camera with the home-built spectrometer

Image analysis (wavelength and Intensity calibration)

The image calibration process begins with the dark calibration, where the intensity is subtracted from the obtained raw images. The wavelength calibration was achieved using emission lines from Hg, Ne and Na for the experiments in the range of 400-650 nm. The He-Ne laser (632.8 nm) and green solid-state laser (532 nm) lines were used to derive an instrument resolution of 0.8 nm. The figure 3.13 illustrates an example of resolution calculation based on the spectrometer design and the manual slit openings. The intensity calibration was done via a halogen lamp of known intensity. The data from the 532 nm laser and halogen lamp are shown in Figure 3.13. The corresponding pixel-to-wavelength conversion is done on the basis of the wavelength data from Hg, Ne, Na, and C_2 lines in the visible region. The CMOS sensor quantum efficiency (shown in 3.12) in the 450-650 nm spectral range was taken into account in the intensity calibration of the spectrum.

The raw spectra exhibit fringes due to optical etaloning. The removal procedure starts with the measurement of blackbody emission of a halogen lamp as a source, ensuring that the spectrum exclusively contains features

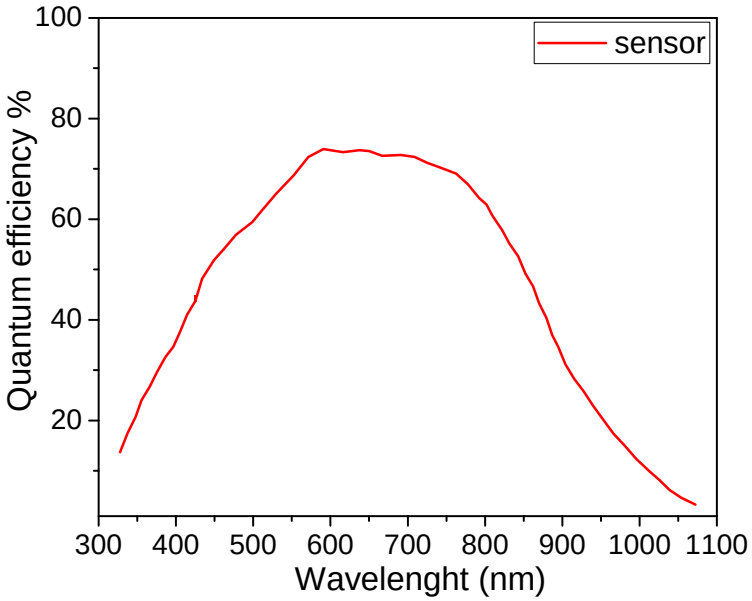


Figure 3.12: Quantum efficiency of NECTA monochrome sensors.

Table 3.1: Theoretical data based on Exocross simulations for comparison of C_2 lines in the spectrum.

(nm)	**Δ V = +1 vibronic transition**	**(nm)**	**Δ V = 0 vibronic transition**	**(nm)**	**Δ V = -1 vibronic transition**
473.71	(1,0)	516.52	(0,0)	563.52	(0,1)
471.52	(2,1)	512.93	(1,1)	558.55	(1,2)
469.76	(3,2)	509.77	(2,2)	554.07	(2,3)
468.48	(4,3)			550.19	(3,4)
467.86	(5,4)			547.03	(4,5)
466.87	(6,5)				

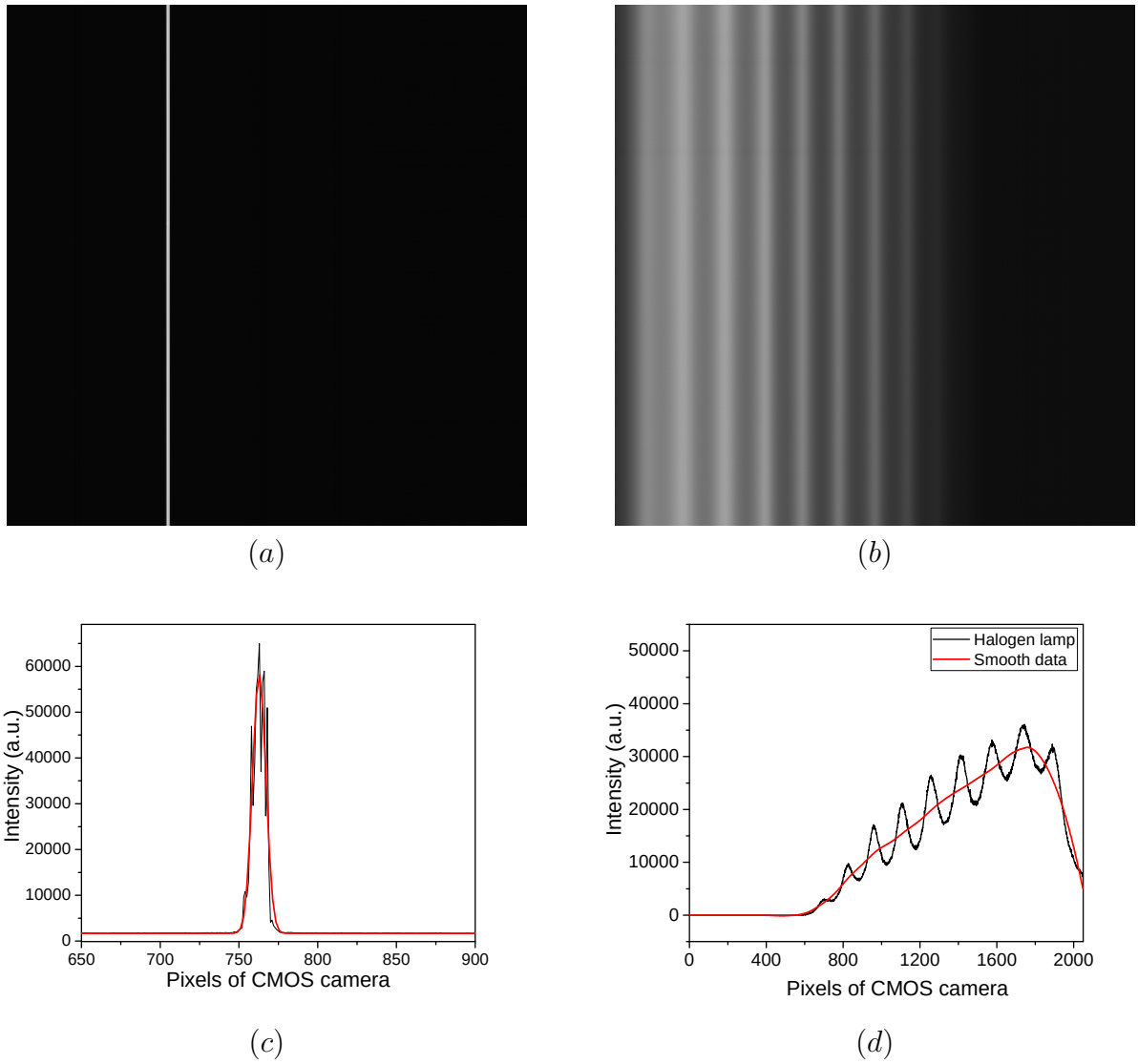


Figure 3.13: Wavelength and intensity calibration (a) Image obtained from a 532 nm laser line ; (b) Image obtained from a halogen lamp source (c) The FWHM of the monochromatic laser light source or other light sources, such as a neon lamp or a mercury lamp, can give the resolution of the spectrometer. The resolution can be controlled by manipulating the slit openings. (Pixel-to-wavelength calibration gives the resolution of 0.8 nm, which is quite suitable for our experiments.) and (d) halogen spectra with pixels is plotted. The data shows an optical etalon present in the spectra.

related to the fringes of the lamp and instrument. We subsequently divide the halogen emission spectra by the Fast Fourier Transform (FFT) of the same spectrum to obtain a scaling factor. A scaling factor for each pixel on the CMOS sensor is then determined and subsequently employed to multiply each freshly obtained spectrum by the instrument, hence yielding fringe/oscillation-free spectra. Custom-written LabVIEW and MATLAB programs acquire the imaging data and handle the task of image processing, such as averaging and background subtraction of intensity. The processed spectra are displayed in Fig. 3.14. The measured spectrum closely corresponds with the literature values in Table 3.1 and the simulated spectrum discussed in Section 3.3.3, suggesting that our spectral resolution is limited by the spatial resolution of the monochromator grating and the area of the CMOS sensor. The time resolution is limited by the electronics of the CMOS camera.

Finally, the novel experimental capability for transient emission spectroscopy, which investigates gas-phase kinetics and spectroscopy, has specific advantages.

1. High sensitivity (capable of detecting CN, CH, C_2, etc.).
2. The system can be easily modified with a change of grating, mirror, slits, or camera according to the requirements.
3. UV–VIS-NIR spectral region coverage.
4. microseconds time resolution.
5. Data acquisition that is efficient, robust, and not sensitive to the position of the optics, as the sensitive optics (grating and mirrors) are housed inside the cover.

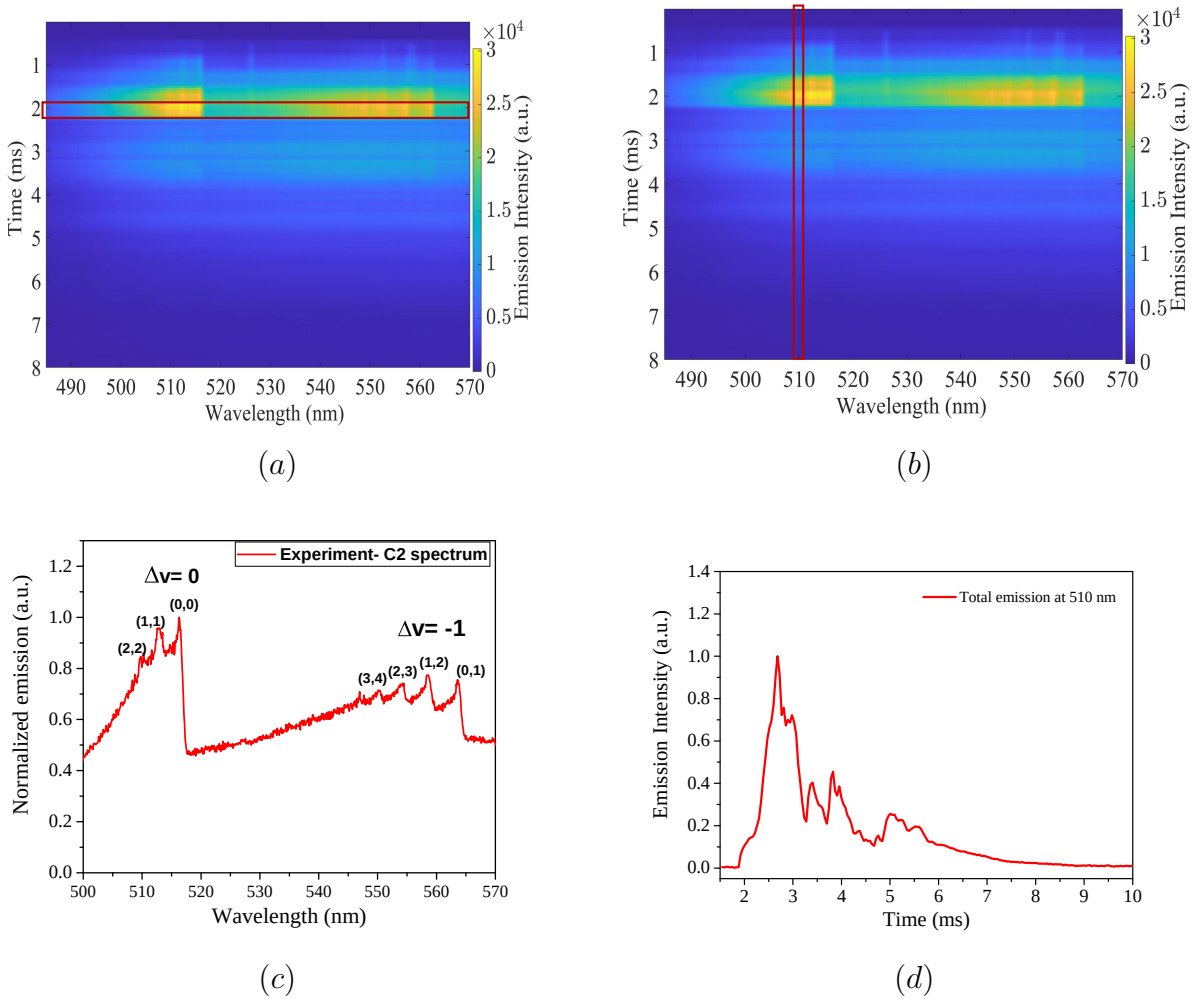


Figure 3.14: Final C_2 (Swan band) — Time-resolved analysis: (a) and (c): 3D image of optical emission (color-coded) versus wavelength (x-axis) and time (y-axis) A slice of the spectra along the wavelength axis is shown below with vibronic transitions from 500 -570 nm ; (b) and (d) 3D image of optical emission (color coded) versus wavelength (x-axis) and time (y-axis) A slice of the spectra along time axis is shown below with time evolution of emission spectra at 510 nm.

6. Modular system that can be applied to any shock tube/tunnel facility in the lab.

3.3.3 Simulation of C_2 emission spectrum

The emission spectrum of C_2 was simulated under local thermodynamic equilibrium using the ExoCross package developed by Yurchenko et al. [206]. ExoCross is an open-access program that simulates absorption and emission spectra, along with various thermodynamic properties, including partition functions and specific heats, derived from molecular line lists. This study utilized the ExoMol molecular line lists for C_2 and the corresponding partition function developed by Yurchenko et al. [207], sourced from the ExoMol database. The details are mentioned in the previous C_{60} [3] paper. ExoCross enables users to incorporate the Lorentzian, Gaussian, or Voigt line broadening parameters, allowing the simulation of the absorption cross section while accounting for the effects of pressure, temperature, or both. Here we used the Voigt profile, as we include doppler broadening (Gaussian profile) and pressure broadening (Lorentzian profile), as the pressure and temperature behind the reflected shocks ranged from 20 to 30 bar and 3000-4000 K respectively.

The Gaussian profile is expressed by the equation

$$f^{G}_{\widetilde{v}_{fi}} = \sqrt{\frac{\ln 2}{\pi}} \frac{1}{\alpha_{fi}} e^{-} \frac{(\widetilde{v} - \widetilde{v}^2_{fi}) \ln 2}{\alpha^2_{fi}}$$

Here $\widetilde{v}_{fi}$ is the central frequency, and $\alpha_{fi}$is the half width at half maximum (HWHM). The parameter α_{fi} is given by

$$\alpha_{fi} = \sqrt{\frac{2RTln2}{M}} \cdot \widetilde{v}_{fi}$$

where R is the ideal gas constant and M the molar mass. In the conducted experiment, the pressure behind the reflected shock is observed to fall within the range of 20 to 30 bar. Consequently, it was necessary to incorporate pressure broadening and utilize a Voigt profile, which is derived from the convolution of Lorentzian and Gaussian profiles. The Lorentzian profile is expressed as

$$f^{L}_{\widetilde{\nu}_{fi}} = \frac{1}{\pi} \cdot \frac{\gamma L}{(\widetilde{\nu} - \widetilde{\nu}_{fi})^2 + \gamma_L^2}$$

where γ_L is the HWHM of the Lorentzian profile, which is given by

$$\gamma_L = \gamma_L^0 \left(\frac{T_0}{T}\right)^{n_L} \frac{P}{P_0}$$

with T_0 and P_0 the reference temperature and pressure set to 298 K and 1 bar, and n_L is the temperature exponent, which has been set to 1. Figure 3.15 illustrates the LTE spectra was simulated within the temperature range of 4000 to 7500 K. The simulated spectra were further convolved with an instrumental function defined by a Gaussian profile, which has a full width at half maximum of 1.4 nm.

3.3.4 Self-absorption effects

Hot and dense media frequently become optically thick and begin to self-absorb. Consequently, emission is significantly influenced by the distortion of the relative intensities of the C_2 bands and must thus be considered [208, 3].

The spectral radiance of a thin segment of C_2 gas of thickness dx can be expressed as

$$dB_{\widetilde{\nu}}(T) = B^0_{\widetilde{\nu}}(T)\sigma(\widetilde{\nu})ndx$$

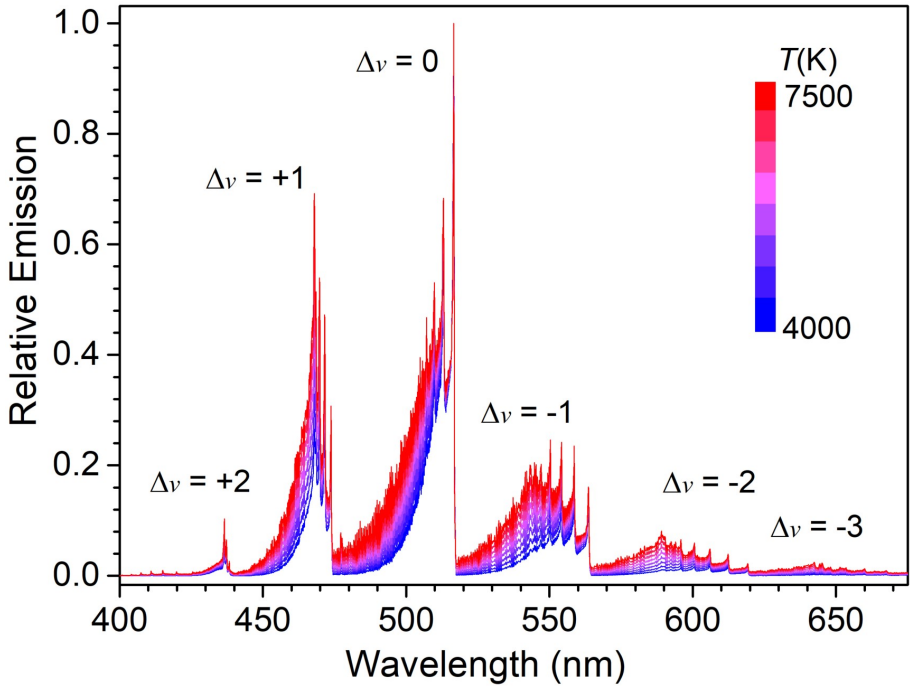


Figure 3.15: Simulated emission spectra of C_2 from 4000 to 7500 K without any convolution. All vibronic bands are labeled.

$\sigma(\widetilde{v})$ the absorption cross section, n is the density. $B^0_{\widetilde{v}}$(T) the blackbody radiance expressed as

$$B^0_{\widetilde{v}}(T) = \frac{2hc^2\widetilde{v}^3}{e^{\frac{hc\widetilde{v}}{kBT}} - 1}$$

By integrating over the column length l for the shock tube, the spectral radiance $B_{\widetilde{v}}$(T) of a column of hot C_2 gas becomes

$$B_{\widetilde{v}}(T) = B^0_{\widetilde{v}}(T)[1 - \tau^{C_2}_{\widetilde{v}}]$$

$\tau^{C_2}_{\widetilde{v}}$, the C_2 gas transmittance, denoted by

$$\tau^{C_2}_{\widetilde{v}} = e^{-\sigma(\widetilde{v})nl}$$

To determine the gas temperature from the C_2 spectral signature, we compare the Δv = 0 and -1 bands simulated for a range of temperatures with the

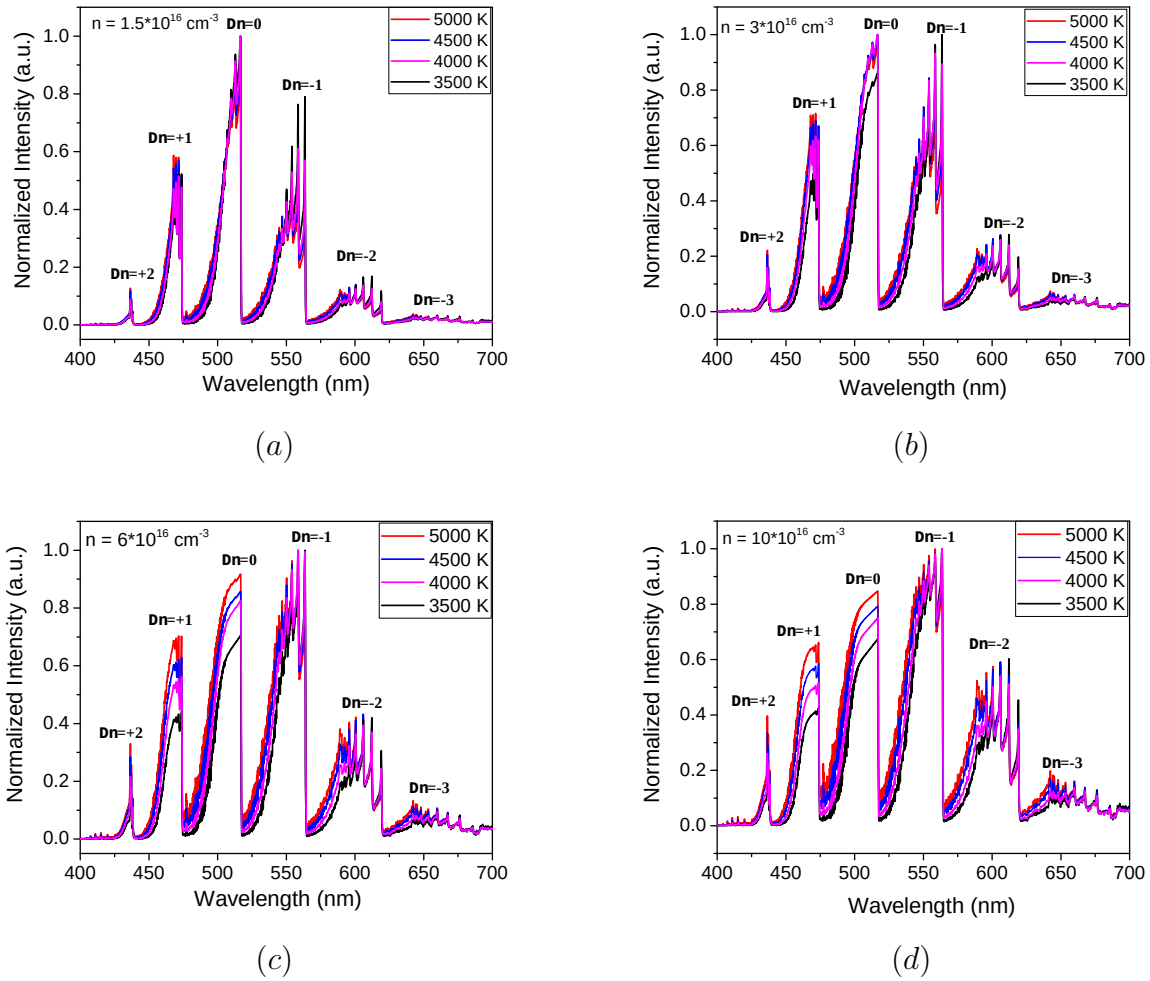
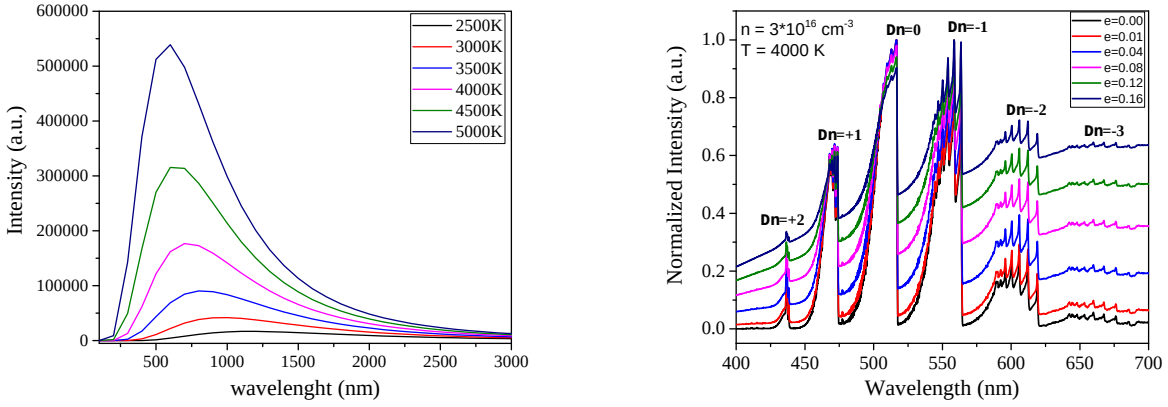


Figure 3.16: Simulated emission spectra of C_2 under LTE approximation including self-absorption for various C_2 gas densities (indicated at the top left of each plot).

experimental spectra. Following the estimation of temperature, an examination of the density of C_2 gas was conducted. The examination of the corresponding band intensity and profile of a series of simulated emission spectra facilitates the determination of optimal matches for C_2 densities.

3.3.5 Broad emission features

All recorded spectra indicate a broad component whose intensity rises with wavelength, reaching a maximum between the wavelengths of 550 and 600 nm. This is attributed to the blackbody emission. The source must derive internally from shock fragments, as the walls of the shock tube do not undergo



(a) (b)

Figure 3.17: Inclusion of blackbody-like emission with C_2 emission corrected for self-absorption; (a) Blackbody emission with temperature; (b) C_2 emission corrected for self-absorption in hot and optically thick medium with blackbody-like emission.

significant heating during the propagation of the shock wave. Consequently, an additional source term must be incorporated into the equation of $dB_{\widetilde{\nu}}(T)$ from a mathematical perspective. Through integration

$$B_{\widetilde{\nu}}(T) = B^{o}_{\widetilde{\nu}}(T)[1 - \tau^{C_2}_{\widetilde{\nu}} \times \tau^{B}_{\widetilde{\nu}}]$$

with $\tau^{B}_{\widetilde{\nu}}$ the transmittance of the broad component. If we neglect the sample reflectivity, we can write $\tau^{B}_{\widetilde{\nu}} + \epsilon_{\widetilde{\nu}} = 1$ with $\epsilon_{\widetilde{\nu}}$ the emissivity of this second component.

3.3.6 Final spectra with simulation

Overall, in our study, we specifically utilize the following relationship to be consistent with the experimental results, along with the addition of a broad Gaussian function between 510 and 580 nm:

$$B_{\widetilde{\nu}}(T) = B^{0}_{\widetilde{\nu}}(T)[1 - \tau^{C_2}_{\widetilde{\nu}}(1 - \epsilon_{\widetilde{\nu}})]$$

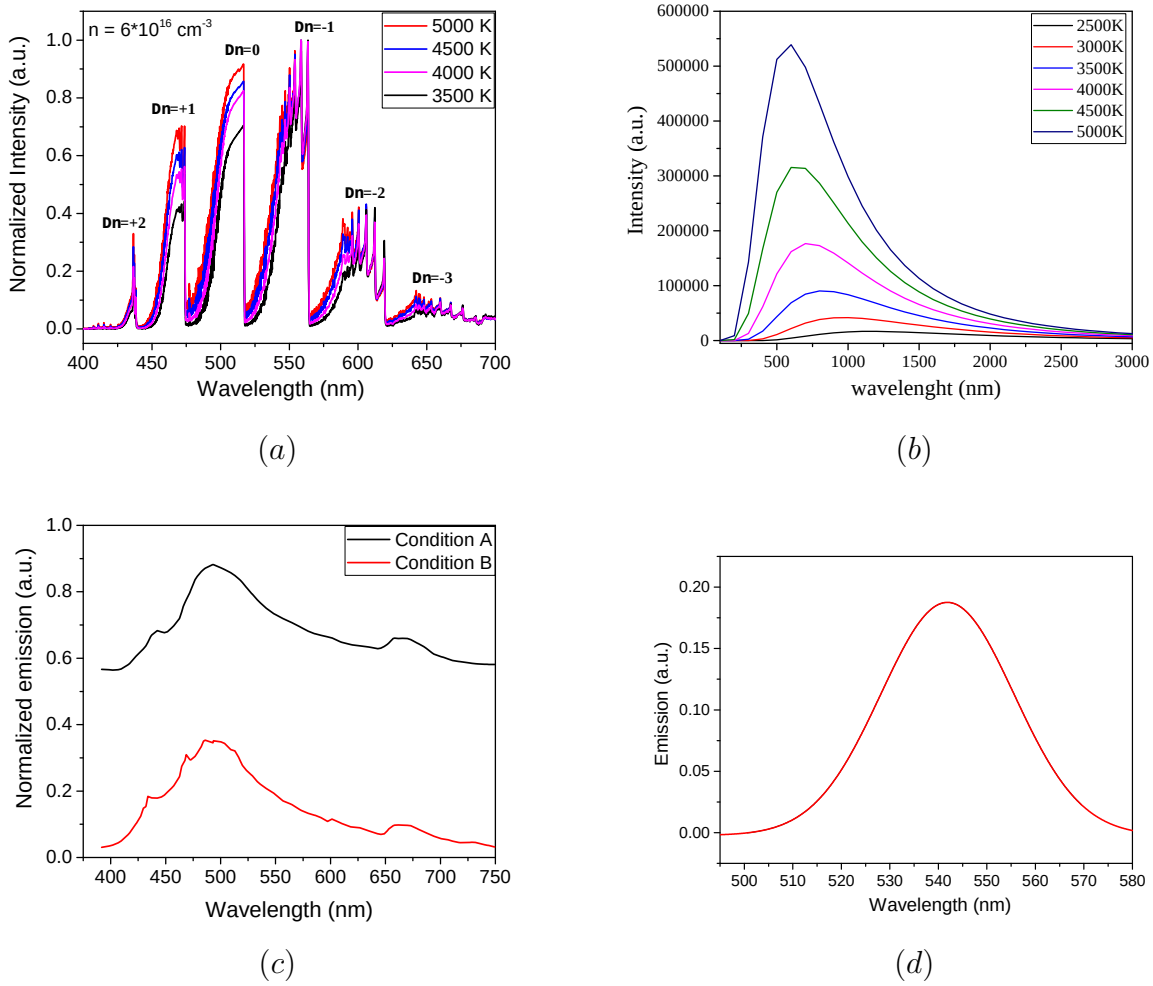
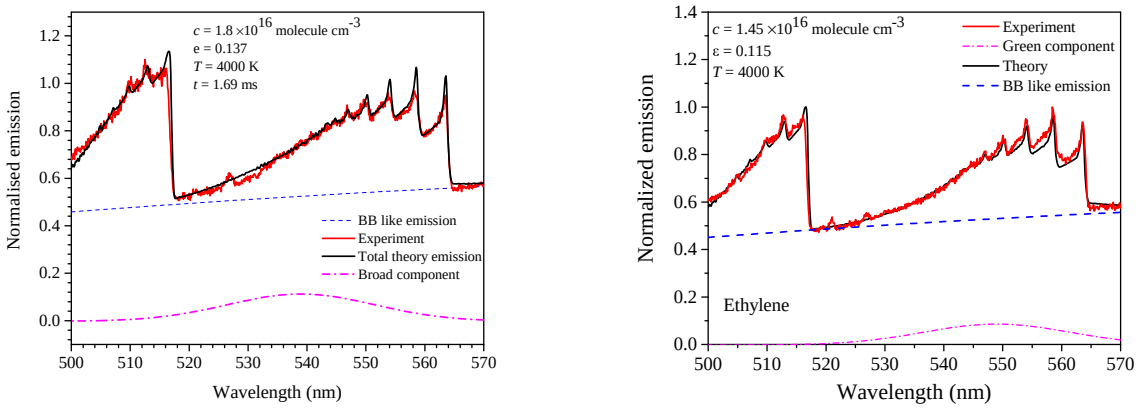


Figure 3.18: The components used in simulations for PAH/hydrocarbon or fullerene shock processing (a) Emission spectra of C_2 corrected for self-absorption in hot and optically thick medium; (b) Inclusion of blackbody-like emission; (c) Example of broad spectra of C_2H spectra (C_2H lines can broaden and shift with pressure and temperature); and (d) inclusion of broad green component (gaussian function)

The total emissivities ϵ_{tot} are adjusted over the 0.05- 0.2 range to reproduce the emission profiles. The three important components for spectra simulation are (see in figure 3.18)

1. C_2 emission corrected for self-absorption in a hot, optically dense medium,
2. The inclusion of blackbody-like emission, and
3. The introduction of a broad green component.

The final spectral analysis for the PAH, hydrocarbon (ethylene), and fullerene



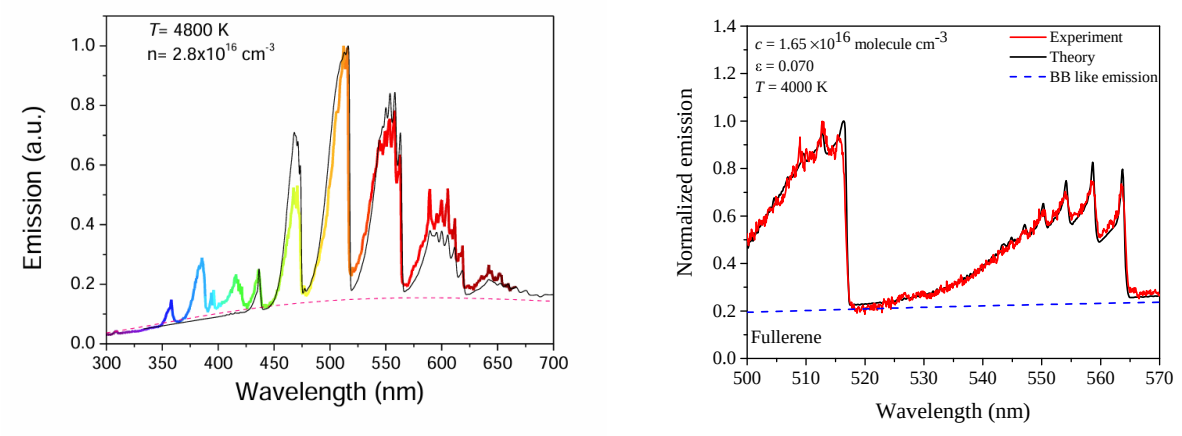
(a) (b)

Figure 3.19: Final spectra analysis: Emission spectra of C_2 corrected for self- absorption in hot and optically thick medium, inclusion of blackbody-like emission and inclusion of broad green component : (a) coronene; (b) ethylene

with hydrogen comprises a total of three variables. C_2 emission corrected for self-absorption in a hot and optically dense medium, the incorporation of blackbody-like emission, and the addition of a broad green component (see fig. 3.19). In contrast, the final spectrum analysis for the fullerene consists of only two variables in total. Emission spectra of C_2 corrected for self-absorption in a hot and optically dense medium, along with the inclusion of blackbody-like emission (see fig. 3.20). The supplementary broad green component is not detected. This outcome is significant as it supports the hypothesis that the green emission originates from small hydrocarbon clusters C_nH_x.

The figure 3.18 shows all the three relevant components and the broad C_2H emission also. The broad C_2H emission spectra and the broad green component are presented together to demonstrate that both components are unique. This is important to understand because based on this we would be able to predict the range of carbon numbers in C_nH_x.

A comprehensive overview is presented in the subsequent section 3.4 that explains every aspect of the emission spectroscopy features.



(a) (b)

Figure 3.20: Final C_{60} fits (Self-absorption with blackbody like emissions was considered in the simulations; (a) Calculated spectra (black) compared to experimental optical emission spectra (colored) of shock-induced C_{60} [3]; (b) Calculated spectra (black) compared to experimental optical emission spectra (red) of shock-induced C_{60} (this work).

3.4 *In situ* optical emission spectroscopy

An optical chamber has been specifically designed to perform *in situ* emission spectroscopy in the shock tube. The emission from the shock tube is captured radially 15 mm from the end flange. A pressure transducer is installed at the same position to get accurate pressure information simultaneously.

A first port is connected to an Acton VM-502 vacuum monochromator from Princeton Instruments with a 200 μm diameter optical fiber to acquire time-resolved emission at a single wavelength. The monochromator covers the 200–600 nm wavelength range and is equipped with a DA-780-VUV photomultiplier tube (PMT). A second port is connected to a STS-UV Ocean Optics mini-spectrometer with the help of a 50 μm diameter fiber. The optical emission spectra result of integrated signals over 5 ms covering the whole shock process. Finally, a third port is connected through a 1000 μm diameter optical fiber to a new home-built time-resolved spectrometer which includes a refurbished manual monochromator and a high-speed camera. The spectrometer disperses the emission from the shock-heated reaction mixture, and a CMOS line camera

records the temporal data of the spectrally resolved emission. The refurbished monochromator was utilized to collect a small wavelength window of light from the emission in the shock tube and supply it to the camera. It is composed of a Newport 77298 grating derived from the Ebert-Fastie concept, employing a single large spherical mirror to collimate point light entering the input port and to concentrate the diffracted light from the grating at the output port. The analysis primarily relies on time-resolved spectral measurements that are rich in spectral information.

The optical emission spectra were acquired through signal integration over a duration of 10 ms for all optical setups. This duration exceeds the time interval during which the gas remains uniformly hot, typically 2-3 ms, and extends into the cooling phase within the test section. Gas samples at different temperatures were subsequently analyzed. The temporal data is acquired from the time-resolved spectrometer. The time-integrated information is obtained from the integrated optical emission spectra. Additionally, a single-wavelength data set is obtained from the VM 502 monochromator.

3.4.1 Integrated optical emission spectroscopy

The emission spectra of shock-induced processing of coronene were collected by the STS-UV microspectrometer integrated for the whole shock duration (10 ms) for a variety of shock conditions (Fig. 3.21). The C_2 signature and the blackbody-like emission clearly increase with temperature T_g. Self-absorption is clearly affecting the C_2 signature. Contamination by sodium (Na I), iron (Fe I), and aluminum (Al I), originating from the surface of the shock tube and diaphragm, was also identified. The PMT signal shown in the Fig 3.22. is taken from the monochromator, where the central wavelength is fixed at 516

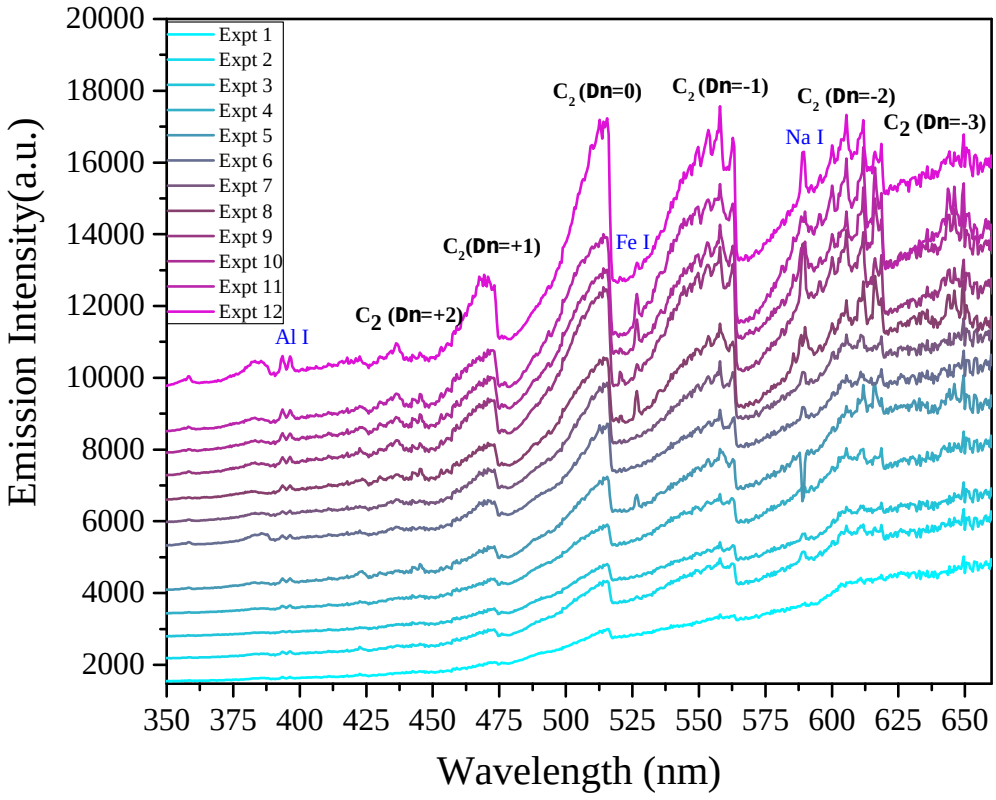


Figure 3.21: UV–Vis integrated emission spectra recorded with the STS-UV Ocean Optics minispectrometer of shock-processed coronene. The spectra were recorded under shock conditions, sampling the T_g=2500-4000 K temperature range.

nm. The total emission signal recorded is similar to the timed emission signal shown in Fig 3.26.

3.4.2 Spectral acquisition, treatment, and analysis

The transient wavelength-resolved emission measurements are collected onto the array of CMOS sensors under a frame acquisition mode. A 42.3 μs resolution has been selected to acquire the timed data from the CMOS line camera. The choice of the camera's frame rate was based on factors such as the readout intensity, readout noise, and dark noise during very short integration times. The recording sequence comprises a matrix of time and wavelength data, as shown in Fig. 3.24. A spectral coverage of almost 100 nm was achieved in the

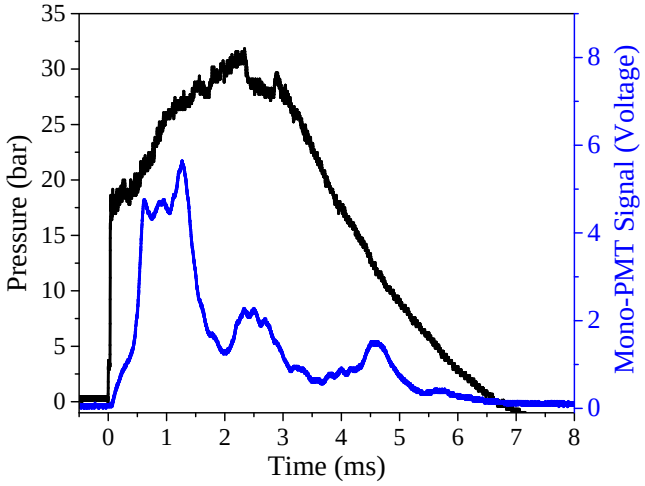


Figure 3.22: PMT signal from shock products recorded at 516 nm at 15 mm from the end flange with the pressure trace measurement. Because of the short distance from the end flange, the incident shock front is barely distinguishable.

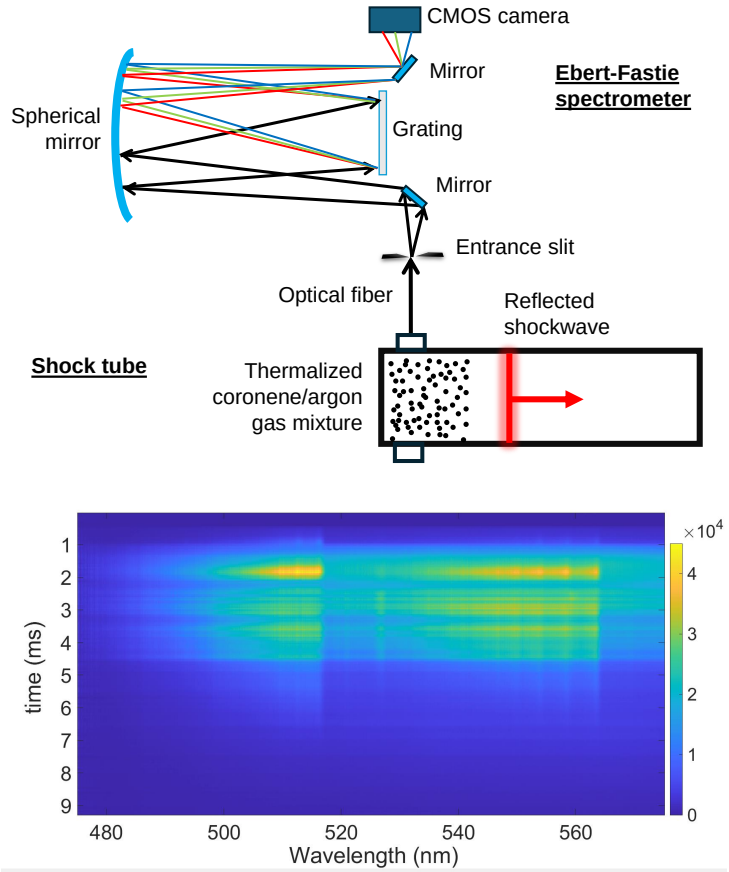


Figure 3.23: Optical diagnostic set-up details for performing *in situ* optical emission measurements in MST facility behind the reflected shockwave. Optical emission (color coded) versus wavelength (x-axis) and time (y-axis) of Coronene exposed to a shockwave characterized by a temperature T_g =4291 K.

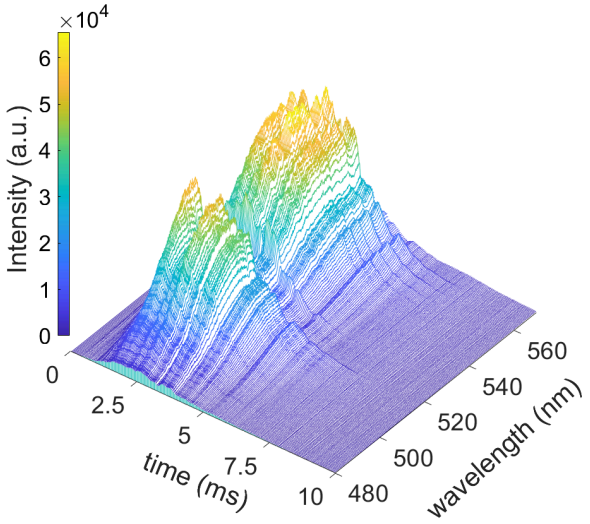


Figure 3.24: Optical emission (color coded) versus wavelength (x-axis) and time (y-axis) from coronene exposed to a shock wave characterized by a temperature T_g of 4291 K.

current experiments. The processed spectra from 0 to 10 ms are displayed in Fig.3.24.

3.4.3 Spectral components and dynamical aspects

A selection of spectra recorded at different times behind the reflected shock was extracted from Fig. 3.24 and exhibited in Fig. 3.25 along with simulated spectra. Specific time stamps were chosen to highlight the evolution of the spectral profile at different intervals behind the shockwave. The interpretation of coronene shock-induced emission components is supported by parallel experiments on corannulene, fullerene, and ethylene. The existence of C_2H and C_nH_x emission could be confirmed or dismissed depending on these interpretations.

As expected for carbon rich species, the *in situ* shock exposure of coronene generates significant amount of C_2 radicals which exhibit a characteristic signature. Figure 3.21 gathers integrated emission spectra recorded under various experimental conditions that clearly demonstrate shock-processed coronene ex-

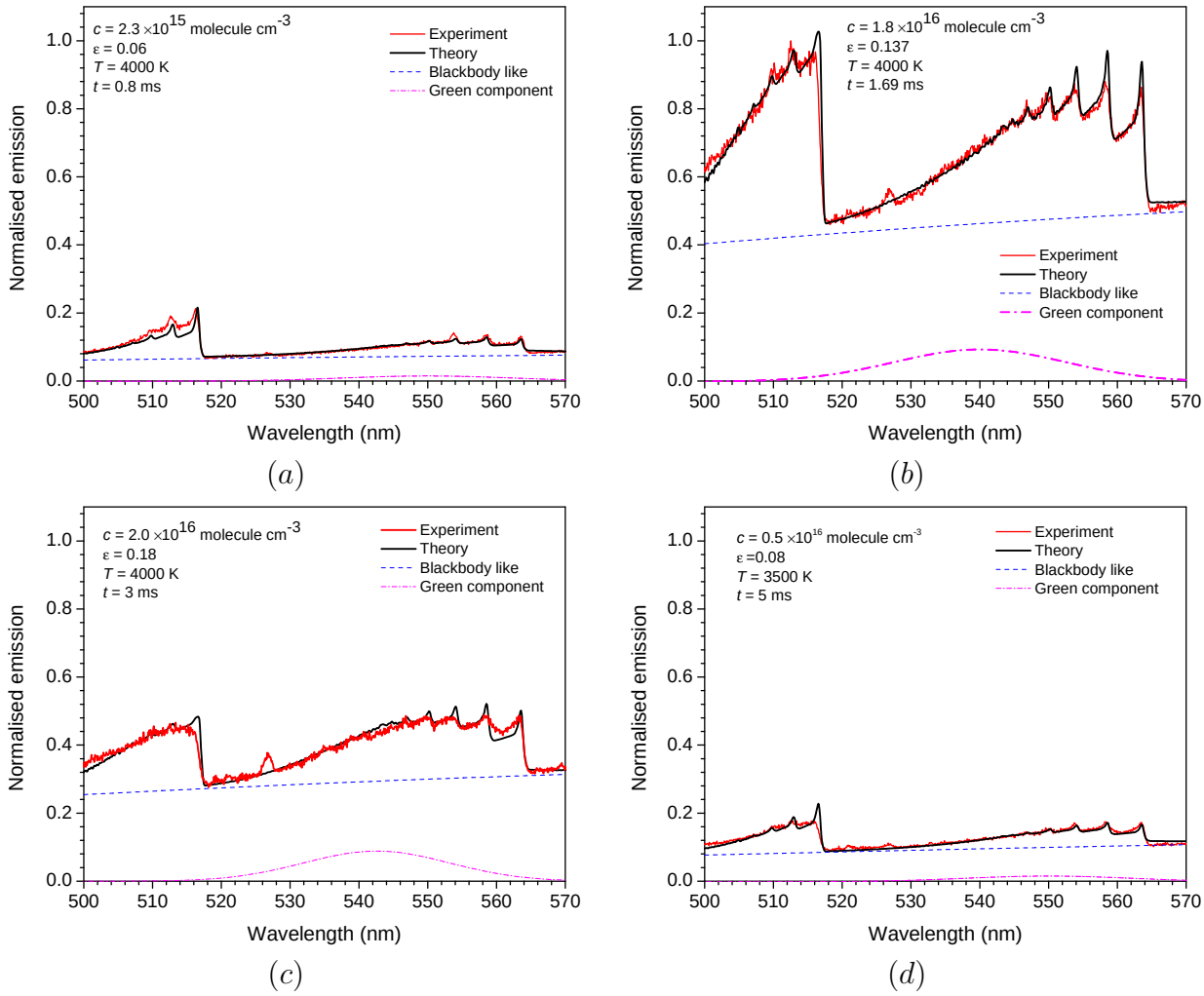


Figure 3.25: Calculated spectra (black) compared to experimental optical emission spectra (red) of shock-induced coronene. Self-absorption was taken into account in the simulations. Adjusted values for ϵ, [C_2] and T_{gas}: (a) 0.06, 2.3×10^{15} molecule cm^{-3}, 4000 K; (b) 0.137, 1.8×10^{16} molecule cm^{-3}, 4000 K; (c) 0.18, 2×10^{16} molecule cm^{-3}, 4000 K and (d) 0.08, 5×10^{15} molecule cm^{-3}, 3500 K. Contamination by Iron (Fe I) (527 nm) was also identified

hibiting C_2 features alongside a broad continuum in the UV-Vis region. Dicarbon C_2 is detected in a variety of astronomical objects, while on Earth it is responsible for the green-blue glow associated with hydrocarbon flames [2]. A detailed discussion of the electronic transitions in the C_2 radical has been presented in the paper [3]. The observed emission arise from transitions between the excited state ($d^3\Pi_g$) and the low-lying electronic state ($a^3\Pi_u$), and are commonly referred to as the Swan bands. Because of the high abundance of C_2 generated behind generated behind the shockwave in our laboratory experiments, its vibrationally resolved bands are strongly affected by self absorption [208].

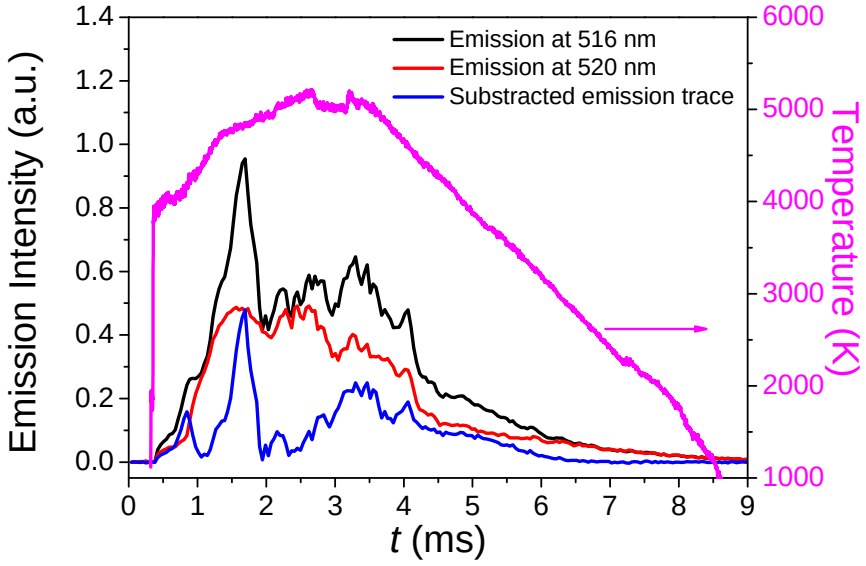


Figure 3.26: Time-resolved optical emission from shock products recorded at 516 nm and 520 nm at 15 mm from the end flange with temperature derived from the pressure trace measurement considering an isentropic compression process $T = \mathrm{c}\ P^{\gamma-1/\gamma}$ with c a constant term. The emission signal at 520 nm falls outside the emission spectrum of C_2, which has a maximum at 516 nm. The difference between the two signals provides information on the emission continuum. Because of the short distance from the end flange, the incident shock front is barely distinguishable.

The time evolution of the emission spectrum is displayed in Fig. 3.24 and covers a wavelength range of$\sim$90 nm. The experimental spectra are normalized with respect to the highest intensity observed, i.e. at 1.69 ms in the

case exposed. A closer examination reveals that the blackbody contribution is minimal for times shorter than 1 ms. However, beyond 3 ms, the blackbody relative contribution becomes more significant. As illustrated in Fig. 3.25 (b), the blackbody contribution accounts for 40% of the highest signal observed at 1.69 ms. This behavior is intriguing and contrasts with our previous study on fullerene C_{60}, where the blackbody contribution did not exceed 10 % of the entire signal. In that case, the blackbody emission was due to the formation of various carbon clusters while in the case of coronene, contribution from both carbon clusters and hydrocarbons is expected. This hypothesis is further discussed in Secs. 3.4.7–3.4.8.

Notably, our work enables an accurate determination of the gas temperature from the C_2 emission spectra, providing improved precision compared to estimates derived from the Rankine-Hugoniot shock equations. We note that the gas temperature is constant between 0.8 and 3 ms and starts to fall after that (Fig. 3.26). Our study is also unique because it gives us direct access to the concentration of C_2 which turns out to vary in the 10^{14}– 2×10^{16} molecule cm^{-3} range. The higher limit, which corresponds to a mass fraction of 7 % with respect to the coronene initial amount, is fully consistent with molecular dynamics simulations (Sec. 3.6).

3.4.4 Minor contribution of CH

The CH radical has well-known emission features at 431 nm ($A^2\Delta$ – $X^2\Pi$), 390 nm ($B^2\Sigma^-$– $X^2\Pi$), and 314 nm ($C^2\Sigma^+$ – $X^2\Pi$) through some of which, it is commonly detected in combustion flames [209] and in diffuse clouds. Noticeably, CH can be employed as a C-shock tracer [210]. In our laboratory experiments, a weak CH emission feature is observed at 431 nm in the STS

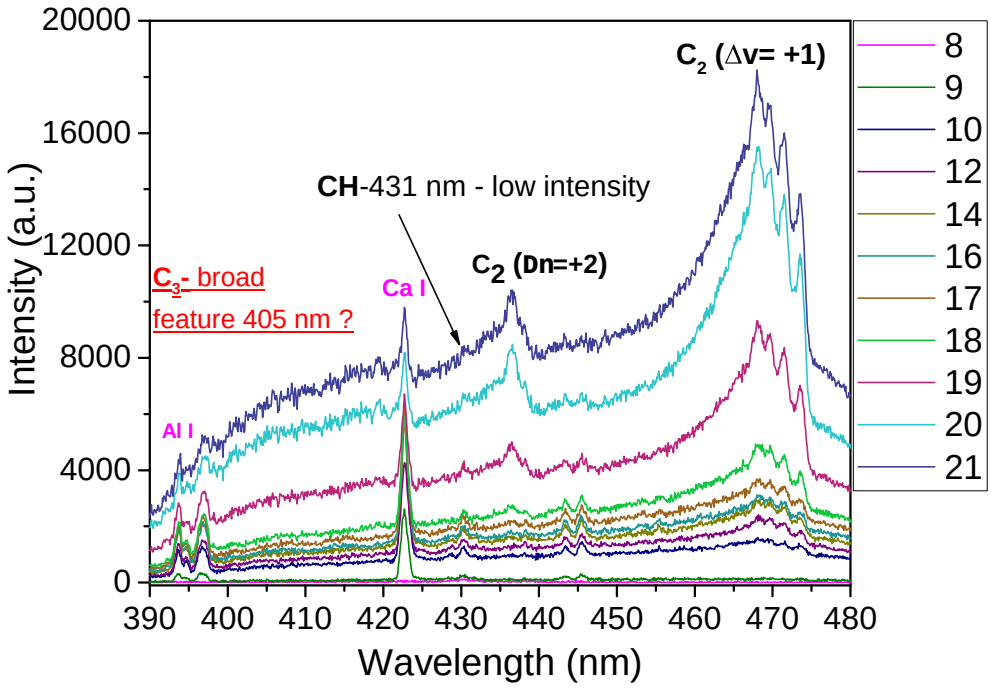


Figure 3.27: Timed emission data recorded from the 390-480 nm wavelength range for shocked coronene at T_g= 4000 K. The right legend are the time steps (42.3 microseconds)

integrated spectra and in the time-resolved spectra. It is superimposed on a broad underlying continuum. The CH emission is observed through time-resolved spectra (see fig 3.27) just behind the shockwave for a millisecond or so, then overshadowed by the underlying blackbody continuum.

Molecular dynamics simulations, discussed in Sec. 3.6, also indicate that the CH species is present in smaller quantities at temperatures above 3500 K. CH fragments arise either from CH-loss in intermediate species or from recombination of C and H atoms ejected during coronene dissociation. Although DFT calculations show CH-loss is a minor pathway compared to H-loss, it can become competitive at higher internal energies [82]. The faintness of the emission feature prevented us to investigate its time dependence.

3.4.5 Absence of C_3 emission

One of the surprising findings of this current study is the absence of C_3 emission (see fig. 3.27). C_3 has been detected in many astrophysical objects including comets in visible emission, circumstellar shells of carbon-rich stars by infrared measurements [211] and dense interstellar clouds in the millimeter-wave region [212]. C_3 has been identified in the laboratory, along with C_2, in e.g. carbon plasmas [213] through its Swings bands at 405.1 nm which correspond to transitions in the $A^1\Pi_u$– $X^1\Sigma_u^+$ system. Notably the oscillator strength for this transition is similar to the $d^3\Pi_g$–$a^3\Pi_u$ transition for C_2 [214, 215].

In our laboratory, C_3 is predicted to be generated behind the shock according to MD simulations detailed in Sec. 3.6. The latter point to the significant production of C_3 above 3500 K mostly generated through the dissociation of larger C_n or C_nH fragments. This is in line with collision-induced dissociation and photodissociation studies which find that the C_3 is an important fragment of carbon chain targets.

Several leads have been explored that could explain the absence of C_3 emission; not to be confused with the absence of C_3. Before addressing them, one should keep in mind that the nature of the emission spectrum of C_3 which is expected to be broad and would therefore remain difficult to be fully distinguished from the broad underlying continuum measured in our experiments, even if present. The first avenue examined relates to collisional relaxation. The absence of C_3 emission in the 405 nm region may be attributed to several factors: collisional quenching, the broad emission characteristics of the C_3 molecule, the generation of C_3 in triplet states, non-radiative transitions, and alternative pathways for C_3 formation during shock processing [216].

The compressed reaction zone behind the reflected shock wave contains vaporized PAHs and rare gas atoms at high temperatures (∼4000 K) and pressure (∼30 bar), in contrast to various previous C_3 spectroscopic investigations that were generally performed at lower temperatures and pressures. Laser-induced fluorescence (LIF) studies demonstrated that the population of the $A^1\Pi_u$ state can drop considerably due to collisions with surrounding rare gas atoms [217]. This is not the case for C_2 which seems much more immune to collisional quenching, although the pressure range explored remains limited. The current experimental conditions therefore support a major role played by collisional quenching, leading to a reduction in the strength of the C_3 emission signal. Secondly, the triatomic nature of C_3, compared to diatomic C_2, leads to an increased number of potential energy levels for electron occupancy, hence resulting in a greater number of probable transitions. Only a smaller fraction of electronic energy levels will be then excited. Additionally, C_3 could be generated in one of the triplet states, either in an $a^3\Pi_u$ or $b^3\Pi_g$ excited state. The duration for spin-forbidden decay to the ground state is 20 ms [218], much larger than the emission timescale accessible in the experiment. It is though not necessary for C_3 to be produced in those states, it could also relax non-radiatively to a triplet state. The combination of all these findings provide a reasonable explanation to the intriguing absence of the spectral signature of C_3.

At last we should also consider alternative pathways for C_3 production in the ground state itself in the presence of C and C_nH species through the reactions:

$$C_2H + C \rightarrow C_3H$$

$$C_2 + CH \rightarrow C_3H$$

$$C_3H \rightarrow C_3 + H$$

The initial two reactions illustrated proceed through barrierless additions of C and CH to C_2H and C_2, respectively, yielding C_3H intermediates. C_3H immediately leads to the formation of C_3 and H by an exothermic reaction [219]. Such neutral reaction pathways may represent only a small fraction of C_3, as the major amount is expected to arise from the dissociation of C_n fragments, followed by recombination reactions as described by molecular dynamics simulations in Sec. 3.6.

3.4.6 Elusive C_2H contribution

The ethynyl radical, C_2H plays a crucial role in the carbon chemistry of astrophysical environments. It can also serve as a proxy for C_2, which is undetectable in the millimeter wave frequency range due to the absence of a permanent electric dipole moment [220]. Besides, the ethynyl radical C_2H is a key intermediate in various combustion-relevant reactions, including pyrolysis and oxidation processes of hydrocarbons, and is an important intermediate of the thermal decomposition of acetylene at elevated temperatures. It plays a crucial role in the formation and destruction of carbon compounds, including carbon chain molecules C_nH as demonstrated by reaction mechanisms identified during the pyrolysis of acetylene [221, 222]. Dispersed fluorescence spectra (continuum emission) of the $A^2\Pi$– $X^2\Sigma^+$ system of the C_2H radical within the wavelength range of 400 to 750 nm have been observed in acetylene pyrolysis experiments [223].

Molecular dynamics simulations of coronene breakdown behind the shock, fully detailed in Sec. 3.6, suggest that C_2H species are produced in significant

quantities, comparatively to C_2 at temperatures below 3000 K. Despite the expected presence of C_2H, its emission signature is not observed. Figure 3.18 illustrates an example of the broad spectra of C_2H along with the other emission features. Despite the fact that the C_2H lines may broaden and shift due to pressure and temperature variations, the figure distinctly illustrates that the broad green component and the C_2H emission are different. The most likely hypothesis is that the C_2H broad features cannot be distinguished in the laboratory experiments because of other underlying constituents in the observable window (500–570 nm) at elevated shock tube temperature and pressure. Because of the lack of oscillator strength values, we are unable to provide an upper limit relative to C_2.

3.4.7 Blackbody-like emission component

Optical emission spectra systematically and clearly reveal a broad continuum whose intensity slightly increases with increasing wavelength (Fig. 3.25 and 3.29). We tentatively attribute it to two principal components. This section is devoted to the first and more prominent component which covers several hundreds of nm, starting from 400 nm and peaking at wavelengths greater than 650 nm according to integrated optical emission measurements recorded over the 300–650 nm spectral range (see figure 3.21 and the discussion in the section 3.3.5 with figure 3.17). This continuum can be easily reproduced by a blackbody-like source and is assigned to the collective emission of carbon C_n and hydrocarbon C_nH_x clusters. The emissivity of blackbody-like emitters varies throughout time, dependent upon the concentration of the large carbon-rich clusters. Section 3.6 can be referred to for more details on the formation of such clusters. Some arguments to support the claim that carbon clusters

are responsible for this emission were provided in the previous study [3].

We discuss further observations hereafter that would lead to including hydrocarbon species in the pool of emitters.Time cuts were performed and examined for ethylene C_2H_4, coronene $C_{24}H_{12}$, fullerene C_{60} and C_{60}/H_2 mixtures. The time-resolved emission signals are superimposed on the temperature profile to highlight the characteristics of the heating and cooling phases. The temperature is derived from pressure traces measurements considering an isentropic process. A more precise value of the gas temperature can be obtained from the analysis of optical emission spectra (see fig.3.29). Figure 3.28 shows that the ratio of the blackbody-like emission over the total emission reported at 516 nm, f_B, markedly increases with the hydrocarbons H/C ratio, and including the eventual hydrogen gas addition (Table 3.2).

For coronene $C_{24}H_{12}$, f_B is about 0.62, more than four times higher than for fullerene C_{60} which is around 0.15. The addition of large amounts of hydrogen H_2 to an initial mixture containing C_{60} at the level of H/C~ 360 leads to almost a doubling of f_B. These two findings suggest that the emitters contain hydrogen. The hydrogen-to-carbon (H/C) ratio for fullerene in hydrogen experiments is determined in the gas phase, assuming complete conversion of C_{60} to C_2 upon thermalization. A known quantity of initial C_{60} (in mg similar to coronene) and hydrogen gas is introduced into the sample chamber. The low C_nH_x component observed in this experiment can be attributed to the substantial loss of hydrogen with carbon, which occurs through the formation of smaller hydrocarbon products, as explained in the ex situ analysis section (see Section 3.7.1 for L2MS comparison between coronene and C_{60} with hydrogen).

The C_2 time profiles look similar except in the case of shock-induced processing of ethylene C_2H_4 for which it is more extended, suggesting a prolonged

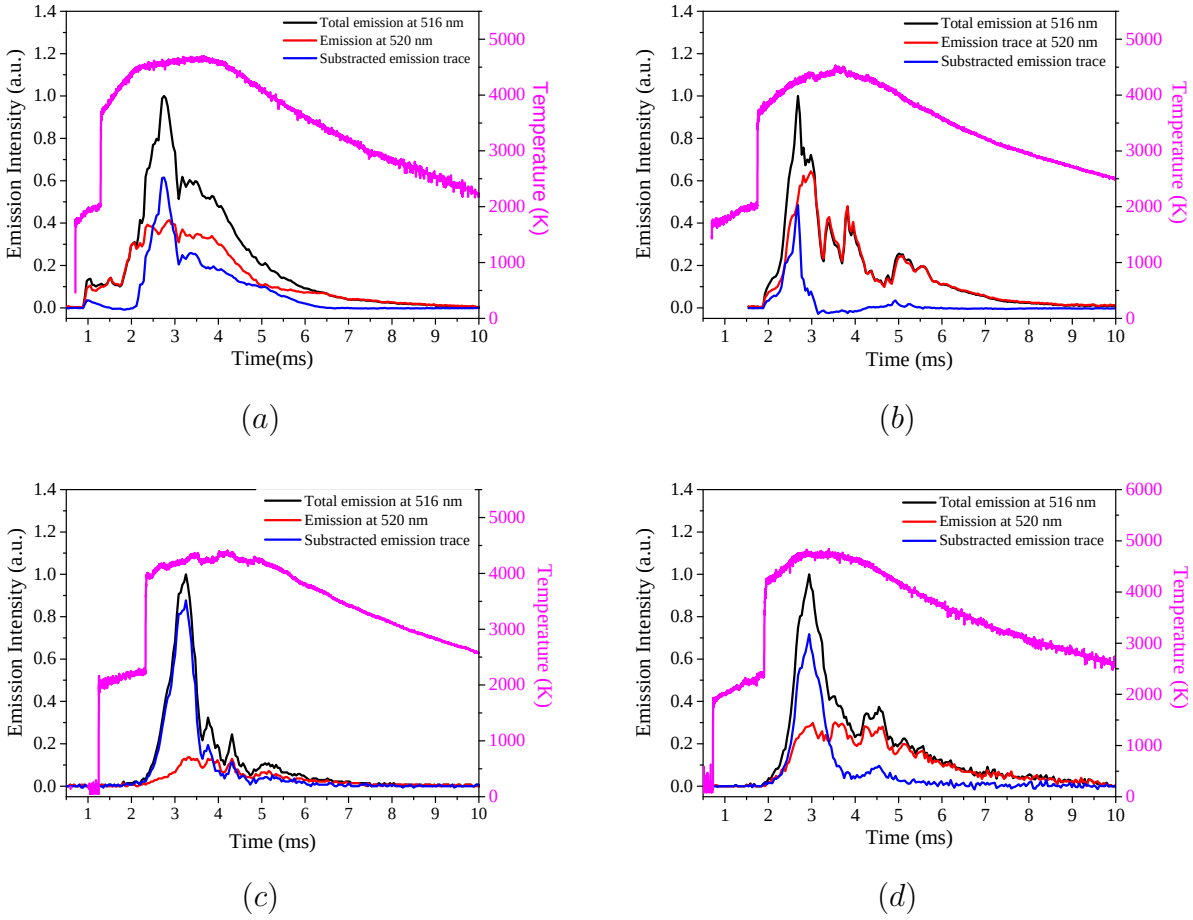


Figure 3.28: Time-resolved optical emission from shock products of different samples at 516 nm and 520 nm with temperature derived from the pressure trace measurements considering an isentropic process. This has been normalized with respect to the maximum intensity wavelength in each experiment. Furthermore, normalization simply enables the comparison of their individual contributions across numerous experiments.(a) ethylene C_2H_4; (b) coronene $C_{24}H_{12}$; (c) fullerene C_{60} and (d) fullerene C_{60} mixed in hydrogen H_2.

production. The blackbody like component spans almost 10 ms, extending well into the cooling phase which typically starts at 4–5 ms. Notably it starts with the incident shock for ethylene, suggesting a rapid formation from C_2H_4 even at the low temperature of $\sim$ 2000 K.

The blackbody-like emission fraction f_B does not show a clear dependence on the number of carbon atoms of the sample as it increases going from ethylene to corannulene and coronene before dropping for fullerene. One of the more robust findings is that the incorporation of H is strongly expanding the variety of emitting species.

Table 3.2: Contribution of the blackbody component to the total emission and C_2 number density derived from time-resolved emission plots of the shock-exposed targets: PAHs (coronene, corannulene), ethylene, and fullerenes (with and without hydrogen) at T = 4000 K. The fraction f_B is the blackbody like emission over the total emission at λ =516 nm and at the time for which the total emission is maximum.

Species	f_B	**H/C**	**C_2 (cm^{-3})**
C_2H_4	0.38	2	1.5×10^{16}
$C_{20}H_{10}$	0.50	0.5	1.9×10^{16}
$C_{24}H_{12}$	0.62	0.5	1.8×10^{16}
C_{60} ; H_2	0.27	360	1.3×10^{16}
C_{60}	0.15	0	1.3×10^{16}

3.4.8 Green emission broad component

The spectra, displayed in Fig. 3.25 reveal another broad emission feature peaking in the 540–550 nm region and approximately 25 nm wide. At its maximum, it represents a significant fraction of the emission in the green, about the same as C_2 and typically a third of the blackbody-like component. This green emission component is also observed in the optical signature of shock-products of PAHs such as corannulene $C_{20}H_{10}$ and hydrocarbons such as ethylene C_2H_4 (Fig. 3.29). In the latter case, shock products, generated in the heating phase observed by optical emission spectroscopy, result from bottom-up chemical processes. But most importantly, this broad green component is not discerned in fullerene dissociation experiments while it is showing up in fullerene/hydrogen mixtures (Fig. 3.29). In the former case, only blackbody radiation is seen and attributed to carbon clusters C_n as discussed in Sec. 3.4.7. This is a clear proof that the emitter contains both C and H.

Notably the emission intensity of the green component in C_{60}/H_2 mixtures is lower than that of PAHs (coronene and corannulene) and ethylene. This could be caused by the reduced presence of C_nH_x clusters. The molecular source of the broad component is challenging to ascertain with existing experimental techniques. Most likely hydrocarbon emitters are discussed in Sec. 3.8

with support from the results from MD simulations and the input from other laboratory works.

3.4.9 Comparison of the time-resolved optical emission spectral measurements

The analysis of coronene $C_{24}H_{12}$ shock-induced optical emission components has been supported by analogous studies on ethylene C_2H_4, corannulene $C_{20}H_{10}$, fullerene C_{60}, and a mixture of fullerene and dihydrogen C_{60}/H_2. The optical emission spectra are displayed below in the Figure 3.29 for the time at which the emission is at its maximum intensity for comparison. Simulated spectra behind the reflected shock at T=4000 K are also reported. Except for fullerene, the optical emission spectra all exhibit a green emission component in addition to the C_2 signature and to the blackbody-like emission. Additionally, the blackbody component is the lowest in C_{60}, which is due to the distribution of large C_n and C_nH_x clusters in the presence of hydrogen.

3.5 Intramolecular vibrational energy redistribution (IVR)-studies

We can gain insight into the energy transfer among various vibronic states in the C_2 Swan band by the vibrational relaxation rate constants (experimentally determined decay constants) and biexponential mathematical fittings.

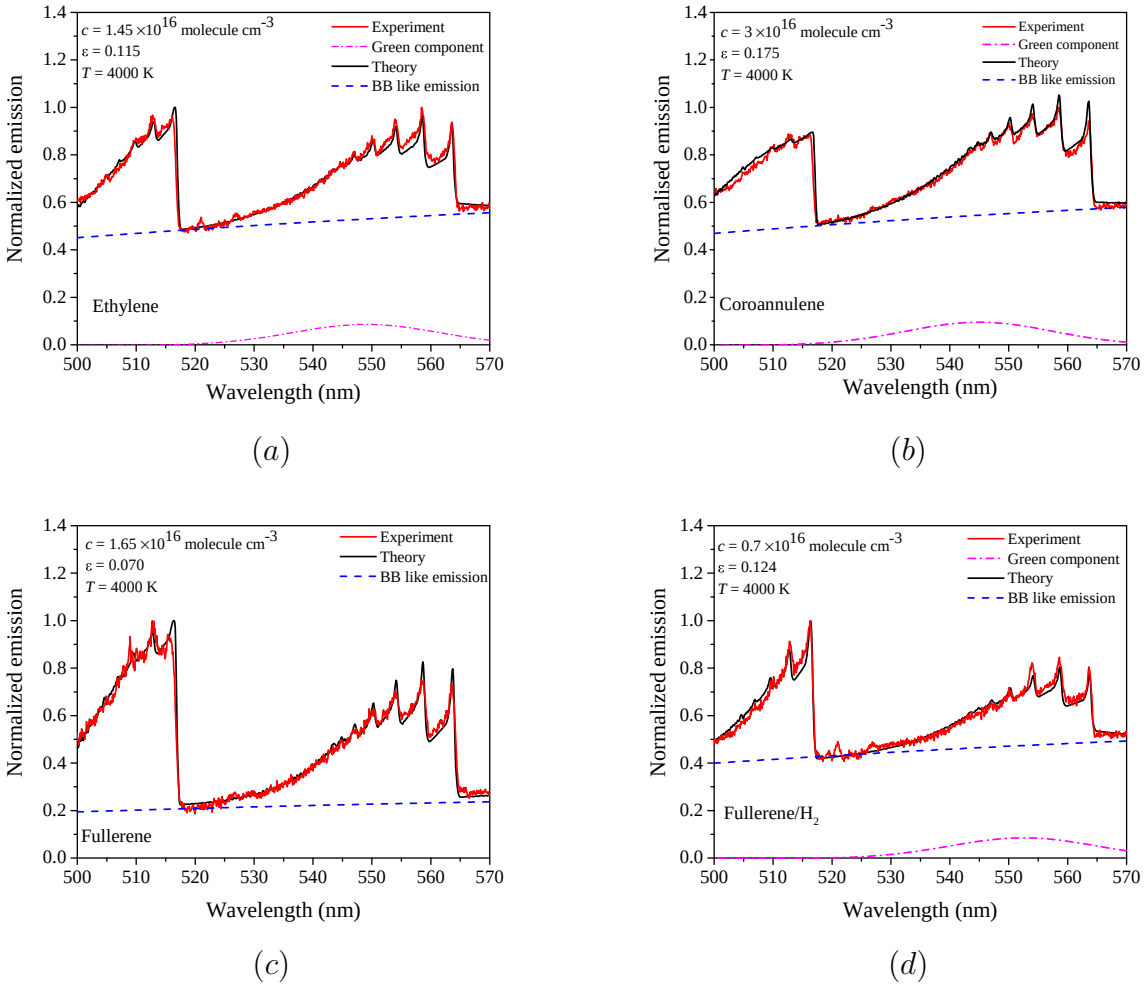
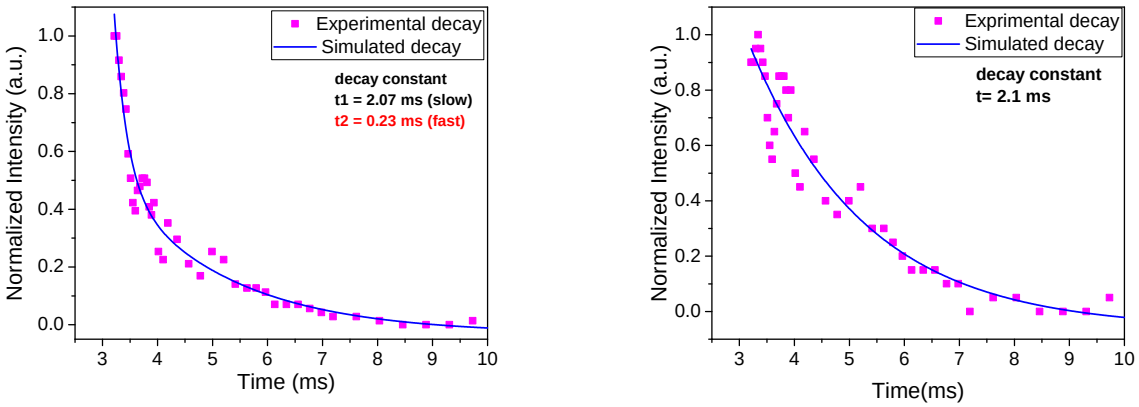


Figure 3.29: Calculated spectra (black) compared to experimental optical emission spectra (red) of shock-induced analogues. Self-absorption was taken into account in the simulations. Adjusted values for ϵ, [C_2] and T_{gas}: (*a*) Shock-induced processing of ethylene C_2H_4 at 4000 K; (*b*) Shock-induced processing of corannulene $C_{20}H_{10}$ at 4000 K; (*c*) Shock-induced processing of fullerene C_{60} at 4000 K and (*d*) Shock-induced processing of fullerene C_{60} mixed with H_2 at 4000 K. Contamination by Iron (Fe I) (527 nm) was also identified .



(a) (b)

Figure 3.30: Exponential fits of the decay component.(a) The plot shows experimental decay data points vs. the biexponential fit for 516 nm. The plot shows that the total decay component is a sum of a slower and a faster decay component;(b) The plot shows experimental decay data points vs. the exponential fit for 520 nm.

Figure 3.30 illustrates an example of the decay profile compared to the exponential fits of a time-resolved emission plot. The biexponential fits validate the existence of two components in all the Swan band transitions (refer to table 3.3). The fits show that there are two components (one faster and the other slower component) responsible for the decay profile of C_2. To validate our fitting analysis, a fit at 520 nm (without C_2 peaks) is also reported, demonstrating a single exponential fit with only one component, having a decay constant similar to that of the slower component. One hypothesis is the faster component is related to the C_2, while the other, slower component is related to the blackbody component.

Table 3.3: Intramolecular vibrational energy redistribution (IVR) process for C_2 lines (biexponential fits).

(nm)	**Vibrational band (ΔV= -1)**	**Decay constant (Biexponential fits) y = A1*exp(-x/t1) + A2*exp(-x/t2)**
563.52	**(0,1)**	**t1 = 2.07 ms (slow), t2 = 0.23 ms (fast)**
558.55	**(1,2)**	**t1 = 1.90 ms (slow), t2 = 0.24 ms (fast)**
554.07	**(2,3)**	**t1 = 1.96 ms (slow), t2 = 0.22 ms (fast)**
550.19	**(3,4)**	**t1 = 2.03 ms (slow), t2 = 0.23 ms (fast)**
(nm)	**Vibrational band (Δ V= 0)**	**Decay constant (Biexponential fits)**
516.52	**(0,0)**	**t1 = 2.18 ms (slow), t2 = 0.24 ms (fast)**
512.93	**(1,1)**	**t1 = 2.47 ms (slow), t2 = 0.24 ms (fast)**
509.77	**(2,2)**	**t1 = 2.37 ms (slow), t2 = 0.23 ms (fast)**
520	**No Transition peaks**	**t = 2.1 ms**

This requires further theoretical studies related to IVR, such as *Master equation simulations in shock wave environment*: For simulating rapidly evolving systems undergoing vibrational relaxation and chemical reaction in a Shock tube the following equations can be used.

1. C_2 (v=0) + Ar = C_2 (v=1) + Ar
2. C_2 (v=1) + Ar = C_2 (v=2) + Ar and so on ...

The consideration of various spin states in the reaction complicates the analysis, necessitating further study.

- **C_2 + C_2 = C_3 + C** (including spin states)

This reaction is crucial for the pyrolysis and oxidation of hydrocarbons (such as acetylene and ethylene) and holds significance in astrophysical systems. While [130] completed a study on rate calculation under different pressure and temperature circumstances, the literature lacks an analysis of dynamics incorporating vibrational states of C_2.

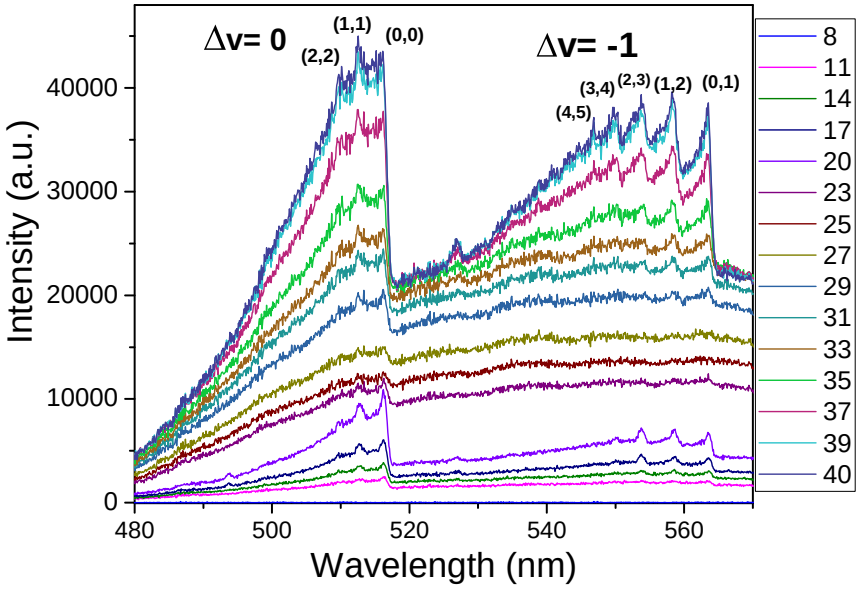


Figure 3.31: Timed emission data recorded from the 480-570 nm wavelength range for shocked coronene at T_g= 4000 K. The right legend are the time steps (42.3 microseconds)

Non-Boltzmann Distribution in Shockwave Interactions: Non-equilibrium conditions may arise if the energy distribution among states does not have sufficient time to equilibrate. Consequently, certain states may exhibit greater population densities than others due to particular reaction dynamics or external factors. One such example is seen in the figure 3.31 where the C_2 band head at 516 nm (0,0) is less intense than the (1,1) transition after a few time steps. This may indicate that higher states exhibit more population density than lower levels for a finite duration. Thus, the IVR study, concerning the transfer of vibrational energy between molecular modes, has major significance.

The MD simulations and ex-situ analysis are essential for understanding all aspects of shock processing of coronene and interpreting the emission spectroscopy results later in the discussion section 3.8. Results have been documented by various contributors, with their names and details included in each section. The material is necessary for a comprehensive discussion and the significance of astrophysical studies in shock tubes. A brief discussion is presented below, highlighting significant results from the various techniques.

3.6 Molecular dynamics simulations

Molecular dynamics (MD) simulations of the dissociation of $C_{24}H_{12}$ have been performed by Aude Simon to help in the interpretation of the results and to gain some insights into the key dynamical processes. This chapter includes a few key results. This study employed an approach analogous to that described in Chakraborty et al. paper [3], with further details provided therein. All simulations were performed with the deMonNano code [224].

The mass fraction contents of the different fragments as a function of time are reported in Fig. 3.32 from 2500-4000 K.

Figure 3.33 below illustrates the formation kinetics of smaller radicals, such as C_2H, C_2, C_3 etc. which are significant for spectroscopy studies at 4000 K. H_2 starts forming within a few hundreds of ps and continues increasing until reaching a plateau. C_2H_2 also starts forming within a few hundreds of ps. Its mass ratio reaches a maximum and then decreases. The same trend is observed for C_2H, which forms in large amounts. Its mass fraction reaches a maximum at 1.6 ns that then decreases to reach a plateau of $\sim$7 % mass. The amount of C_2 keeps increasing to reach a plateau of about 10 % mass. C_3 forms after

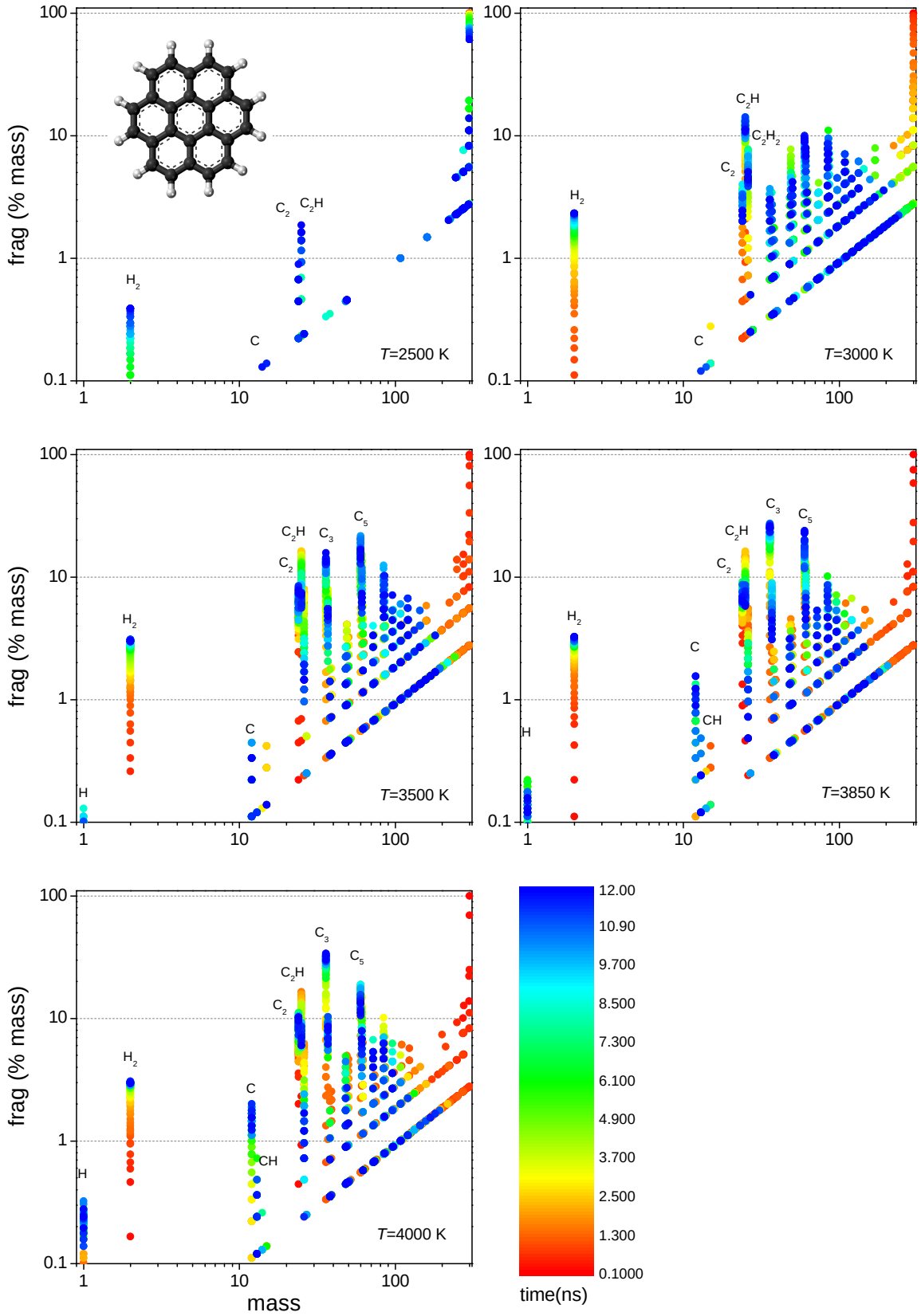


Figure 3.32: Molecular dynamics simulations of the dissociation of coronene in the canonical approximation. The thermalization time was set to 100 ps. The confinement effects were simulated by implementing a repulsive spherical wall with a 60 Å radius. The fragmentation of coronene causes the appearance of a variety of fragments over the 2500–4000 K range *(Figures by Aude Simon).*

1 ns. Its mass fraction increases rapidly up to about 8 ns and then reaches a plateau of about 30 % mass. CH is found in lower abundance but also reaches a plateau of 5 % mass.

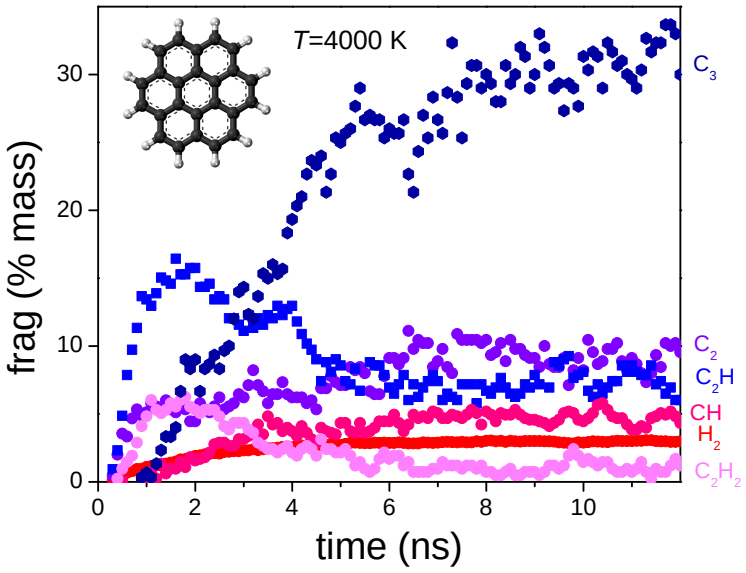


Figure 3.33: The time evolution of shock products of coronene is illustrated here. MD Simulations of the temporal evolution of shock products of coronene at 4000 K *(Figures by Aude Simon)*.

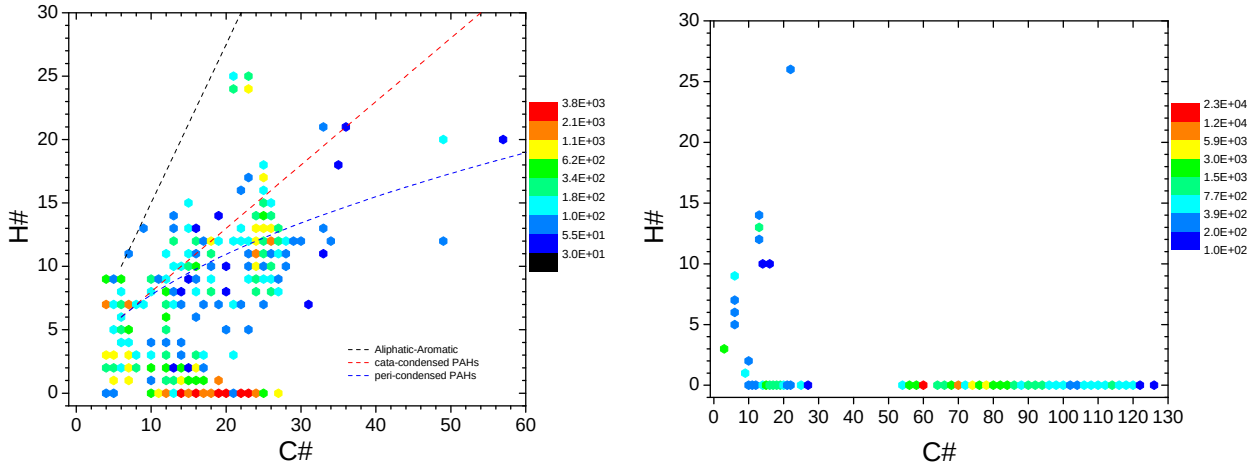
C_3 is present in the simulations and becomes more abundant than C_2 at 3500 K, although it is not observed in the experiments. A deeper insight into a few simulations shows that the formation of C_3 is not direct: it comes from the dissociation of larger C_n or C_nH fragments previously formed after dissociation and recombination steps. Conversely, C_2 can be formed by direct dissociation.

The results of the MD simulations show that the dissociation of coronene leads to the formation of a variety of size distributions of hydrocarbons, depending on temperature, mainly through a top-down process.

3.7 *Ex situ* analysis of solid residues

3.7.1 Laser desorption laser ionization mass spectrometry

Solid residues from a coronene sample exposed to a shock wave were analyzed by Hassan Sabbah using the AROMA setup (Astrochemistry Research of Organics with a Molecular Analyzer) fully described by Sabbah et al. [225].



(*a*) (*b*)

Figure 3.34: Laser desorption laser ionization mass spectrometry analysis of solid residues from (*a*) coronene sample exposed to a shock wave at $T = 3500\,\mathrm{K}$ estimated from integrated emission spectroscopic measurements. The diagram displaying the H# versus the number of Carbon atoms C# is color-coded for mass peak signals (log scale); (*b*) C_{60} in H_2 exposed to a shock wave at $T = 4000\,\mathrm{K}$. The diagram displaying the H# versus the number of Carbon atoms C# is color-coded for mass peak signals (log scale). *(Figures by Hassan sabbah).*

The L2MS mass spectrum (Figure 3.34) is dominated by peaks corresponding to bare carbon clusters and PAHs with mass-to-charge ratios (m/z) below 300. The diagram shows a substantial population of PAHs, mostly pericondensed structures with C# < 24, as well as hydrogenated carbon clusters. The ratio of the combined signal from all $C_{24}H_x$ species, where $8 \leq x \leq 14$, to the total detected signal is 6.5%, suggesting that most of the original material has undergone shock processing. An overall H/C ratio of 0.29 is obtained by integrating the abundances of all detected species down from the initial H/C

ratio of 0.5 (indicating loss in the form of hydrogen as no small hydrocarbon is detected). These results provide clear evidence of the carbonization of coronene when exposed to a shock wave.

Post-shock solid residues from C_{60} mixed in H_2 were mass-analysed to help in the interpretation of the results obtained for other dust analogues. To shed some more light on the processes at play, we compare the present findings with results from our initial study on the shock-wave processing of C_{60} in hydrogen [115] and from complementary L2MS data (Fig. 3.34). Mass spectra show that H is very weakly incorporated into the end-product. Most of the peaks are assigned to carbon clusters. The L2MS mass spectrum of post-shock products from a fullerene/H_2 mixture highlights the presence of two broad groups. The first one dominates and regroups carbon clusters, almost bare, with 50<C#<125, while the second one is dominated by carbon-rich species with C#<30 and a slightly higher hydrogen-to-carbon ratio, but still orders of magnitude less than that of the PAH sample mentioned above. The examination of post-shock gaseous mixtures via gas chromatography confirmed the production of methane (CH_4), ethylene (C_2H_4), acetylene (C_2H_2), and ethane (C_2H_6). Despite an initial H/C ratio of 360, a considerable proportion of carbon and nearly all of the incorporated hydrogen seem to be lost through these minor hydrocarbon pathways. (also evident from the low blackbody contribution in the total emission in the section 3.4.7 for C_{60} with H_2). As a result, the solid residues are made up almost solely of pure carbon material, unlike what is observed for coronene. Notably, by contrast to these results, the coronene post-shock volatiles analyzed using gas chromatography did not reveal the formation of such small stable hydrocarbons.

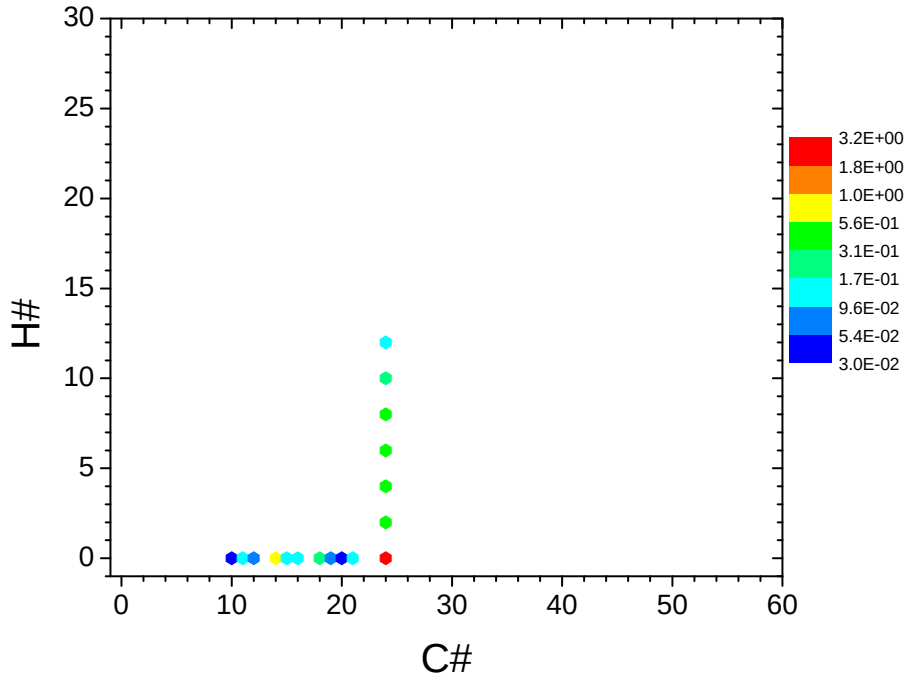


Figure 3.35: Photodissociation mass spectrum of cold trapped coronene $^{12}C_{24}H_{12}^{+}$ under continuous visible UV irradiation of Xe lamp + OPO laser tuned at 480 nm for the duration of 120 s.

3.7.2 UV-photodissociation mass spectroscopy

The following discussion is crucial for understanding the differences between shock processing and UV photodissociation techniques, allowing a comparison of experimental results in the discussion section.

UV photodissociation mass spectra of isotopically pure coronene ions $^{12}C_{24}H_{12}^{+}$ cryogenically trapped in PIRENA (Piège à Ions pour la Recherche et l'Etude de Nouvelles Espèces Astrochimiques) were recorded [81]. The mass spectrum is also represented in a C# versus H# diagram to facilitate comparison with L2MS results. The products of this shock processing differ significantly from those resulting from UV photodissociation (see Fig. 3.35), highlighting that shock-induced processing is a two-step mechanism: first, the initial molecule is broken apart by a high-energy input; then, during the subsequent cooling phase, new chemistry is initiated via the recombination of molecular fragments.

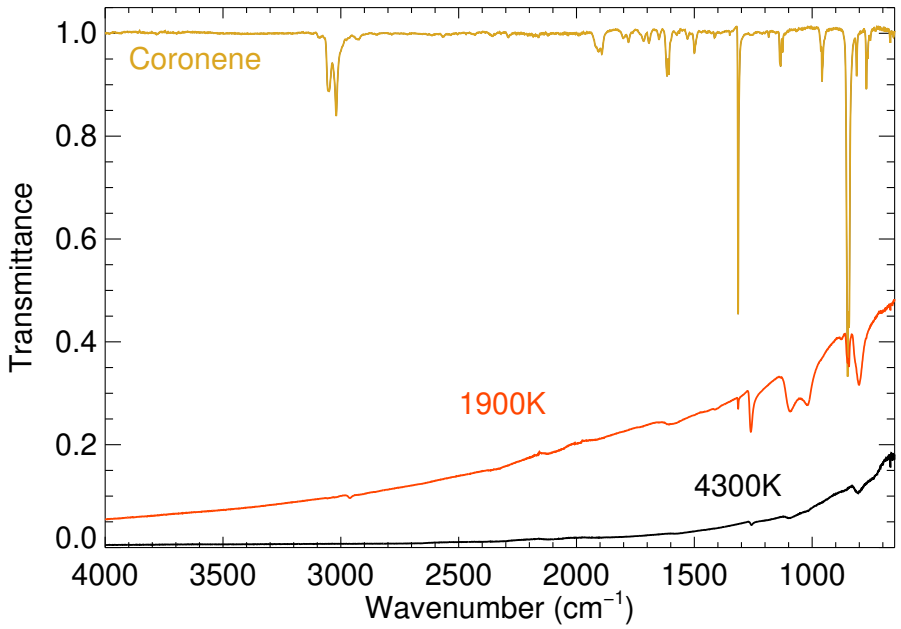


Figure 3.36: Infrared transmittance spectra of the pristine sample (coronene) and shocked coronene at $T_g = 1900\,\mathrm{K}$ and $4300\,\mathrm{K}$. *(Figures by Emmanuel Dartois)*

By comparison of the L2MS data of UV photodissociation and shock processing data, we can infer that, in UV photodissociation, the hydrogen is lost completely, while hydrogen is still present in the post-shock analysis.

3.7.3 IR micro-spectroscopy

Infrared spectra were recorded by Emmanuel Dartois on *ex situ* extracts, flattened sample using a Nicolet infrared microscope. Typical recorded transmittance spectra are shown in Fig. 3.36.The spectra exhibit a gradual attenuation of the molecular vibrational bands as T_g increases, signifying the development of a macromolecular carbon-rich material, alongside the appearance of a strong continuum resulting from the incremental formation of a zero-gap material. The figure may indicate the existence of graphitic or graphene-like carbon nanostructures at 4300 K, further validated by HRTEM images.

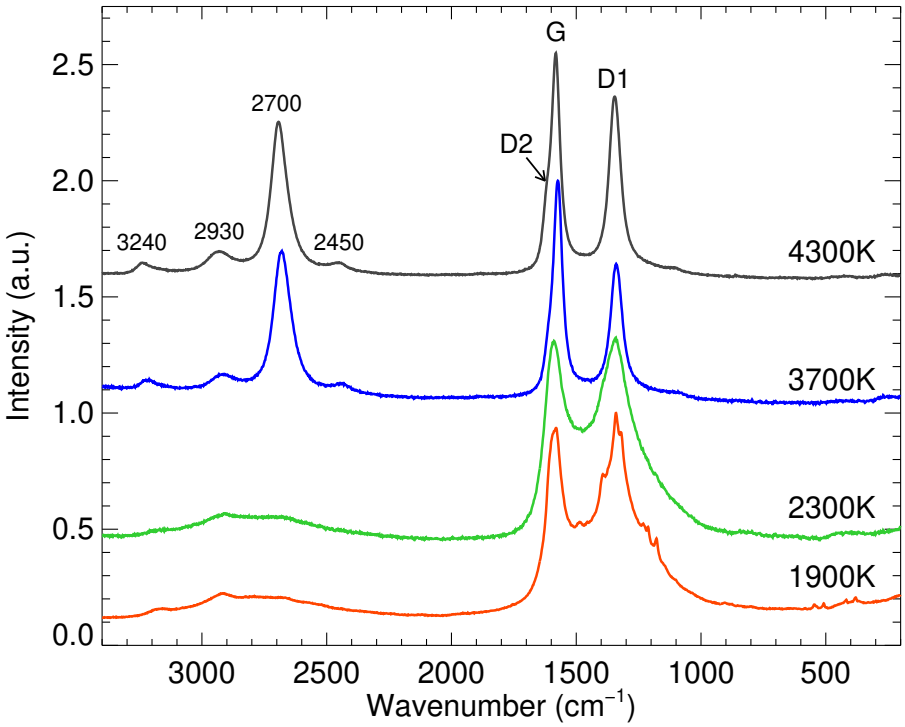


Figure 3.37: Raman spectra of solid residues of shocked coronene at temperatures T_g covering the 1900 K to 4300 K range. *(Figures by Emmanuel Dartois)*

3.7.4 Raman spectroscopy

Raman spectra were recorded by Emmanuel Dartois on *ex situ* extracts, using a DXR Nicolet Raman microscope with a 532 nm laser on the SMIS beam line at the synchrotron SOLEIL.

A selection of spectra is shown in Fig. 3.37.As the temperature increases, the bands become narrower, reminiscent of a progressively more ordered system, close to graphitic. The high T_g Raman spectra also correspond to highly ordered carbon particles, which are confirmed in the HRTEM analysis.

3.7.5 X-ray diffraction

The powder XRD pattern of pristine and shock processed $C_{24}H_{12}$ was recorded at IISc Bangalore by S Ranjan, using Cu Kα radiation source (PANalytical) in the 2θ range from 5° to 90° (Fig. 3.38 shows only the range in which peaks are

obtained). The XRD pattern of pristine coronene was indexed in space group $P21/n$, consistent with previously reported results with unit cell dimensions a =10.122 Å, b =4.694 Å, c =15.718 Å, β = 106.02° [226]. The prominent and intense diffraction peak at $2\theta = 9.30°$ originated from the highly organized arrangement of coronene molecules. The distinct peaks (2θ = 9.30°, 11.62°, 12.03°, 17.39°, 18.17°, and 18.70°) further validated the remarkable crystallinity of the samples.

The exposure of coronene fine powder to a shock wave in Ar gas (T_g =3400 K) leads to a drastic reduction of the intensity of all the diffraction lines, as shown in Fig. 3.38. The XRD pattern displays a broad and weak diffraction peak at approximately 25°, corresponding to the (002) plane reflection of aromatic layers, and a barely visible peak at around 43°, associated with the (100) plane reflection of aromatic layers. The (002) peak in XRD pattern of graphite is attributed to the orientation of the aromatic ring carbon layers arranged in a three-dimensional configuration. The (100) peak corresponds to the extent of condensation of the aromatic ring, specifically the dimensions of the carbon mesh segment of the aromatic structure. The narrower and stronger the (002) peak, greater the orientation of the aromatic layer slice. The narrower and sharper the (100) peak, the greater the size of the aromatic layer slice [227]. The interlayer spacing (d_{002}), the graphitization degree (g), and the crystallite size(L_c) were calculated using Bragg's equation, the Franklin equation, and the Scherrer equation, respectively.

$$d_{002} = \frac{\lambda}{2} \sin \theta_{002}$$

$$g = \frac{0.3440 - d_{002}}{0.3440 - 0.3354} \times 100\%$$

where κ is the Scherrer parameter, β represents the full width at half max-

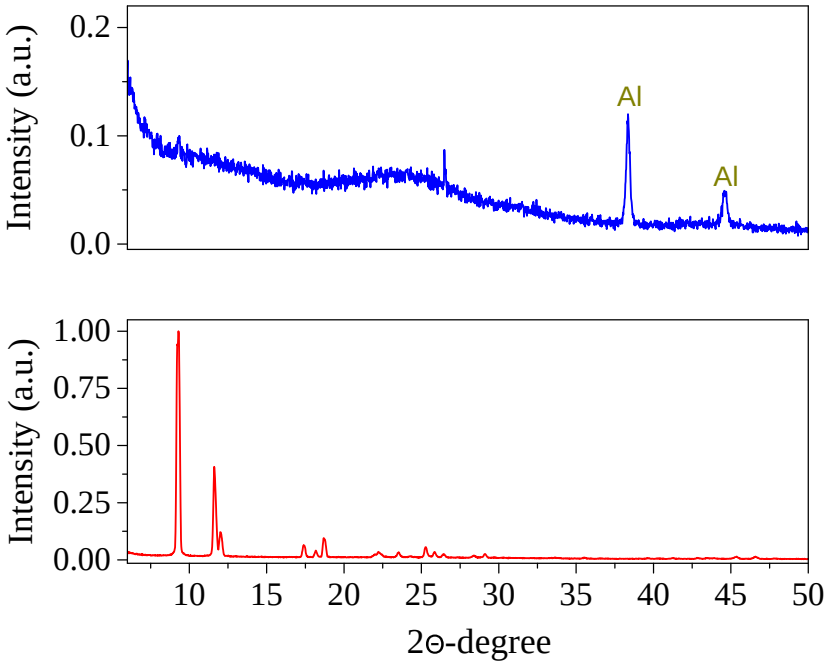
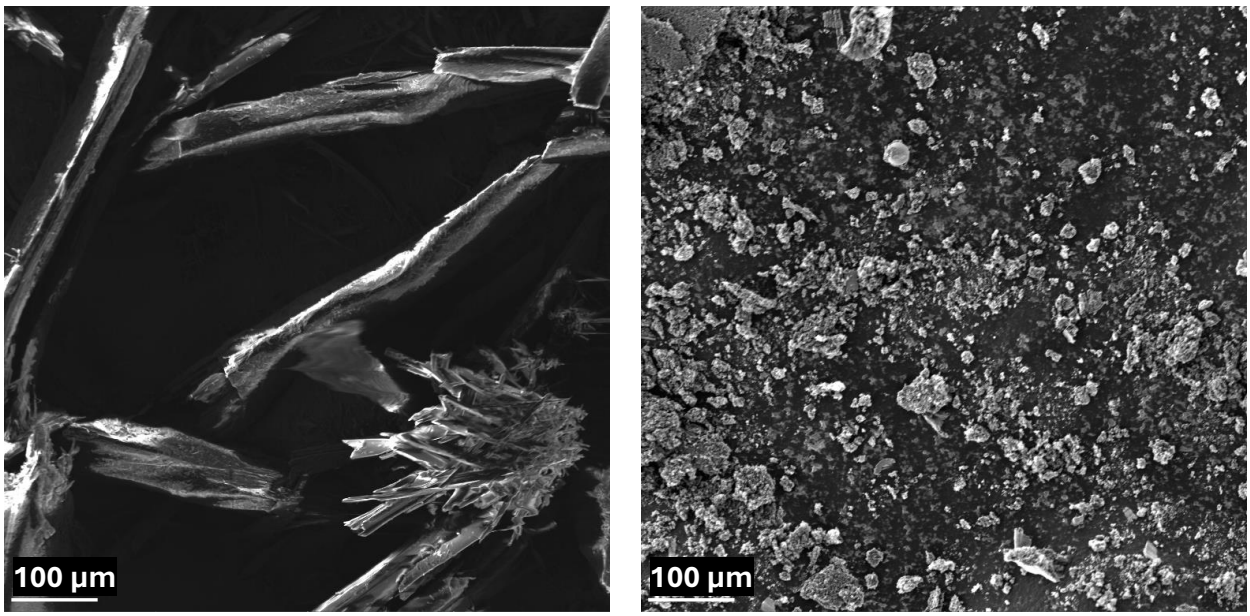


Figure 3.38: X-ray diffraction spectra of pristine (bottom) and shock-processed (top) coronene.

imum (FWHM) of the diffraction peaks, θ stands for the Bragg angle corresponding to the diffraction peak. For the post shock samples the values found are: $d_{002} = 0.34$ nm, $g = 75.7$ % and, $d_{001} = 0.21$ nm. The theory and equations discussed above, along with the XRD results, indicate the presence of graphitic nanosized structures in the post shock sample indicating some degree of graphitization of products. Detailed analysis of the nature and the variation in the composition of shock products can be confirmed further by carbon nanostructures evidenced by HRTEM imaging. The peaks observed at 38.3° and 44.6° following shock exposure result from aluminum impurities originating from scraping off the surface of the aluminum test section during sample collection and from the ruptured diaphragm.

3.7.6 Scanning electron microscopy

Scanning electron microscope (TESCAN, MIRA, FEG SEM) recorded at IISc Bangalore by S Ranjan, was used to study the morphology of coronene and



(a) (b)

Figure 3.39: Magnified SEM images. (*a*) fibrous coronene powder; (*b*) shocked coronene products at T_g= 4370 K; *(Figures by S Ranjan).*

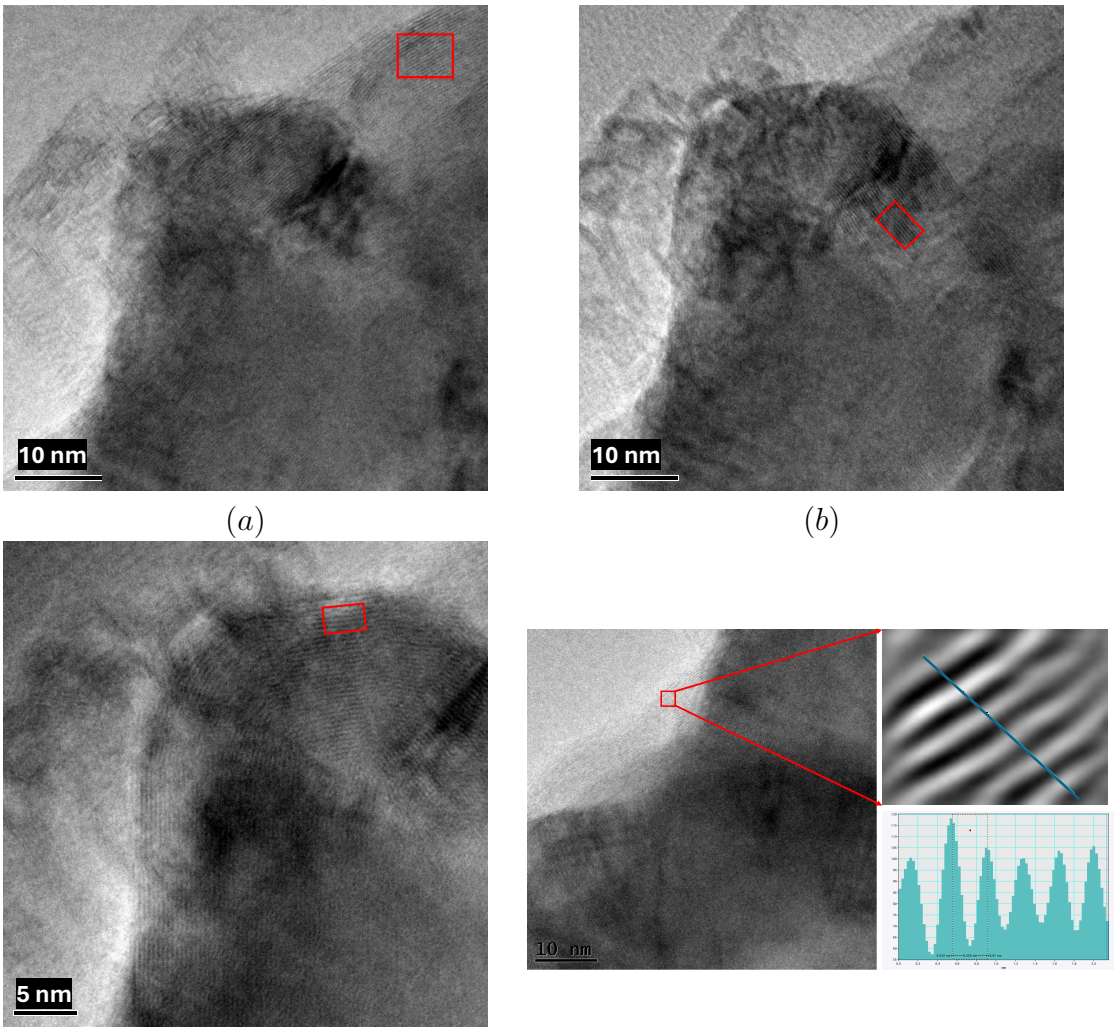
its solid residues after exposure to strong shock waves. SEM micrographs of coronene powder before and after shock exposure in Ar gas were recorded. Figure 3.39 illustrates that the original powder exhibits a structure resembling fibres, whereas the exposed powder exhibits predominantly nanoparticles with spherical shape.

3.7.7 HRTEM imaging

High resolution transmission electron microscopy (HRTEM) recorded at IISc Bangalore by S Ranjan. It was utilized to examine the crystalline and amorphous characteristics of the samples at the nanometer scale. The microscope (T20 ST) at the Advanced Facility for Microscopy and Microanalysis, IISc Bangalore, was operated at 200 kV. The samples were prepared using dilute suspensions of coronene powder before shock loading, and the post-shock sample was collected after shock exposure. The solution was obtained by sonicating particles in ethanol for 30 min and drop cast on separate TEM carbon-coated

copper grids. The studies were carried out on pristine and shock-exposed coronene samples suspended on separate carbon grids.

The bright field image and the electron diffraction pattern of unexposed coronene, provided in the Fig. 3.41, show agglomerated fibres. The selected area electron diffraction pattern (SAED) of the crystalline structure of pristine coronene is also displayed. The TEM images at 100 nm magnification show predominately graphitic layered structures such as nano-onions, nanotubes and nanoribbons (Fig. 3.40). The HRTEM image of exposed sample reveals lattice fringe spacing of 0.359 nm which corresponds to the spacing of graphitic planes as shown by XRD analysis. The SAED pattern of shock-exposed material displays diffuse and symmetrical rings, attributed to the graphitic structure (d_{002}=0.35 nm, d_{001}=0.21 nm also confirmed by the presence of the broad peak in the post shock XRD analysis). Carbon nano-onions or multi-layer fullerenes belong to the fullerene family and comprise closely packed quasi-spherical and polyhedral onion like graphitic layers [228]. Carbon nano-onions were identified in the TEM images as mostly quasi-spherical, exhibiting dimensions between 10 and 150 nm, comprised of concentric graphitic shells. From the HRTEM imaging, it was determined that the interlayer distance is approximately 0.35 nm confirming a graphitic-like structure. Evidence of nanoribbons and nanotubes was also found in the HRTEM imaging with a spacing d of approximately 0.36 nm (within red rectangles in Fig. 3.40). Theoretical studies conducted by Kit et al. [229] have demonstrated the formation of nanotubes through the twisting of graphene nanoribbons. Thermally induced self-intertwining of graphene nanoribbons facilitates the synthesis of carbon nanotubes, [230] and conversely, unzipping of carbon nanotubes can result in the fabrication of carbon nanoribbons [231, 232].



(a) (b)

(c) (d)

Figure 3.40: High-resolution transmission electron microscope images of shocked coronene at Tg= 4370 K showing images of carbon nanostructures with the red rectangle showing the area where the spacing d was measured. (*a*) HRTEM of carbon nanoribbons; (*b*) HRTEM of carbon nanotubes; (*c*) HRTEM of carbon nano-onions; (*d*) HRTEM image of shocked powder with magnified image of the selected area and interplanar spacing of powder along the line mentioned in the image.*(Figures by S Ranjan)*

Our findings are also consistent with, e.g., the work of [58] in which fullerene-like soot generated by laser pyrolysis of C_2H_4/C_2H_6 or laser ablation of a graphite target was observed. In that work the particles result from gas-phase condensation at high temperature ($\geq$ 3500 K). Only low-temperature processing (below 1700 K) led to the formation of PAHs.

3.8 Discussion

The *ex situ* and *in situ* analyses supported by MD simulations are employed to sketch a global scenario of the experimental processing of coronene behind the shock. Our current understanding of the initial steps is that the incident shockwave disperses the coronene fine powder deposited onto the plate holder and mixes it with the gas. The sudden rise in the gas temperature behind the shock leads to a rapid increase in the internal energy of the microcrystals. Individual coronene molecules can then overcome intermolecular forces that weakly bind them. This leads to sublimation. Once in the gas phase, the large number of collisions ensures rapid thermalization of coronene with the argon bath gas on a timescale close to tens of microseconds. The high internal energy of coronene is achieved behind the reflected shock, triggering its breakdown. Strong dehydrogenation and generation of hydrocarbons and carbon clusters follow. When the gas cools, the shock fragments chemically recombine and lead to the formation of carbon nanostructures.

3.8.1 Onset of breakdown: major loss of hydrogen

The fundamental mechanisms of coronene dissociation and the routes that dictate the dynamics, as well as the observation of distinct emission components,

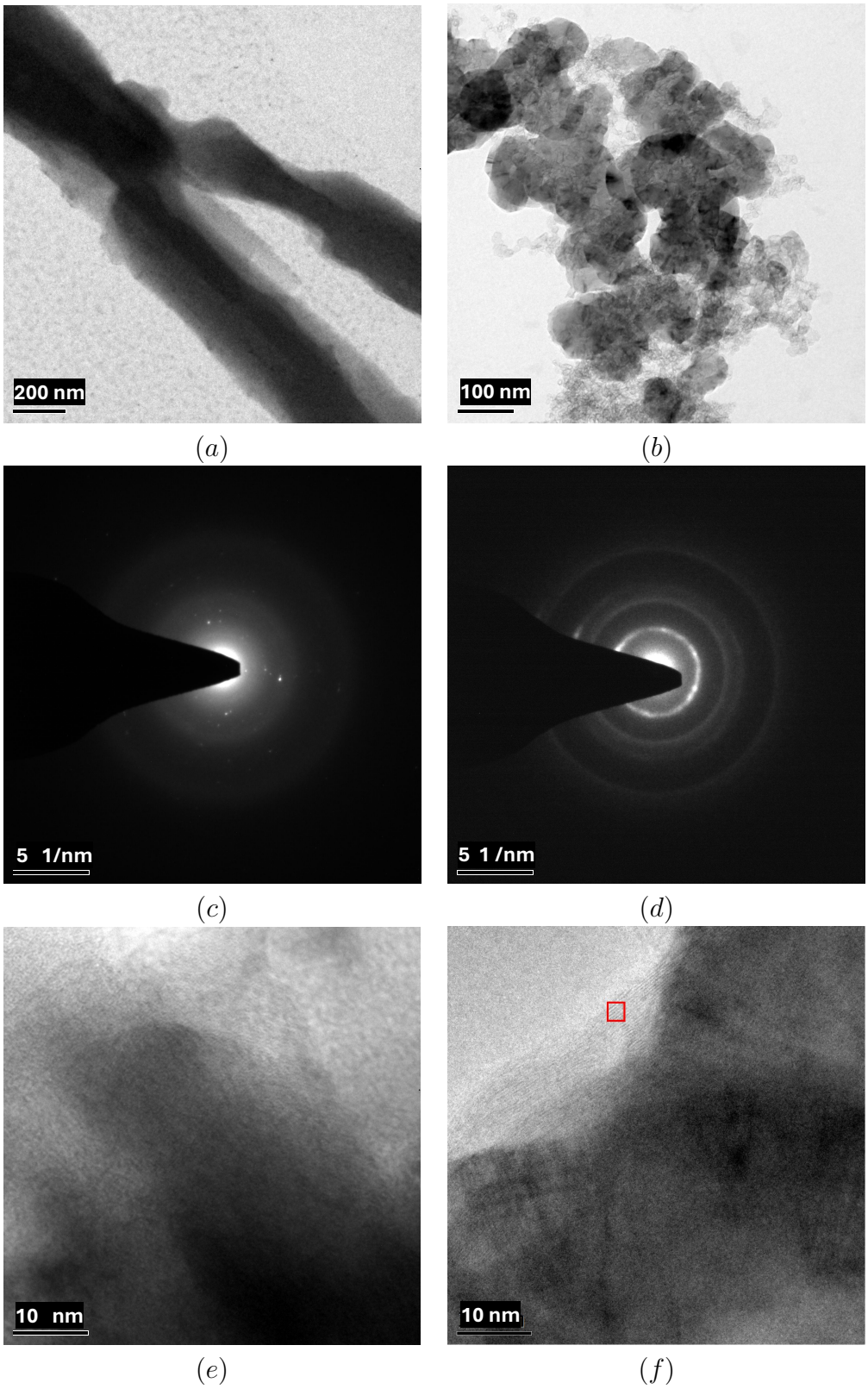


Figure 3.41: TEM images. (*a*) TEM image of coronene organized in fibers at low magnification; (*b*) TEM image of carbon nanostructures at T_g= 4370 K; (*b*) TEM image of carbon nanostructures at T_g= 4370 K; (*c*) SAED pattern of coronene;(*d*) SAED pattern of carbon nanostructures at T_g= 4370 K; (*e*) 10 nm scale HRTEM of coronene;(*f*) 10 nm HRTEM image of carbon nanostructures at T_g= 4370 K. *(Figures by S Ranjan)*

were investigated with a great diversity of methods. However, the interpretation also benefited from additional experiments on the thermal processing of PAHs, ethylene, and C_{60} with hydrogen, which all exhibit a wider variety of pathways than that of C_{60} alone, due to the presence of hydrogen. Major routes include H, H_2, and C_2H_x ejection and their subsequent recombination with other radicals, thereby propagating chain reactions alongside possible low-energy barrier hydrogen abstraction reactions.

One major finding of this work is that the loss of hydrogen plays a pivotal role in coronene dissociation. The dehydrogenation mechanism for PAHs involves unimolecular dissociation at high internal energy, as a result of shock heating. It is understood that, for the internal energy of coronene reached behind the shock, C-H cleavage is favored over C=C cleavage due to a lower energy barrier. The simulations confirm an extensive dehydrogenation with i.e. almost all hydrogen ending up in H_2, close to the maximum mass fraction of 4%, above the temperature of 3500 K. Loss of H is also observed for $T \geq 3500$ K but remains a minor exit channel.

The abundant loss of H_2 observed in our work is consistent with the previous study by Chen et al. [94] , whichshows that loss of H_2 from unimolecular dissociation of PAHs becomes efficient for internal PAH ttemperatures higher than 2200 K for any PAH size and excitation process. Regarding the precise mechanism leading to H_2 loss, that cannot be deciphered with our MD pprocedure; theoretical studies demonstrate that a first hydrogen atom migrates on the edge of the PAH through a roaming process [94, 233] , to attach another carbon atom, forming a -CH_2 aliphatic group from which H_2 is further removed.

3.8.2 Medium-size hydrocarbons, carbon clusters and blackbody-like emission

The emission spectra resulting from the shock processing of PAHs and fullerenes, are primarily characterized by the C_2 signature, accompanied by a broad underlying continuum in the UV-visible region. The latter is assigned to two distinct components. The most intense one, in terms of integrated visible flux, covers a spectral range of hundreds of nm (Fig. 3.21) with blackbody-like behavior and is attributed to medium-size carbon clusters, of the C_n and C_nH_x type. The blackbody-like character of the broad component results from the collective emission of a huge number of molecular species and isomers, whose individual contributions add up and cause specific features to disappear. Obtaining a large number of isomers requires large species. This is a critical point. As an illustration, $C_{24}H_{12}$ possesses 52 213 isomers, with 79% belonging to the family of flakes, and 19% branched [234]. In our previous study on C_{60} shock processing, the extensive underlying emission was ascribed to the blackbody-like radiation from diverse carbon clusters (C_n<40) based on energetic and thermodynamic calculations derived from the simulated collective emission spectra [3]. The ratio of blackbody-like to C_2 emissions observed in shock-processed PAHs and ethylene via optical spectroscopy is significantly higher than that for C_{60} (Fig. 3.17), thereby lending credence to this hypothesis of a second family of emitters of the C_nH_x type, in addition to the first family already iidentified, which gathers large carbon clusters C_n. Although C_2 emission is observed in both fullerene and PAH runs, there are some specifics in the mechanisms ejecting the first C_2 units, which are worth examining.

Remarkably, the rapid heating phase of the shock-induced processing shares some similarities with UV-driven photodissociation. The excitation energy in

a molecule, acquired by photon absorption, is in most cases completely randomized in all its vibrational modes before it is decomposed, and a statistical theory can be used to adequately describe the dissociation dynamics. A few differences can be underlined, though. First, for shocks, the internal energy of the parent, provided by incessant collisions with the bath gas, can be quite high, i.e. $\sim$20 eV for coronene at 4000 K. This is well above Ly-α single photon energy provided by hydrogen lamps but similar to the energy reached in infrared multiphoton excitation schemes. Second, the high internal energy of the reactants and products behind the shock is maintained for a few milliseconds compared to nanoseconds in the case of pulsed irradiation. Shock-induced decomposition is therefore expected to be rather extensive behind the shock wave in the laboratory, hence drastically compressing the astrophysical timescales.

Early ion trap photodissociation studies on compact PAHs show that the bare C_{24}^+ carbon cluster emerges as the predominant component following complete dehydrogenation of $C_{24}H_{12}^+$ but also the less compact species naphtho[2,3-a]pyrene $C_{24}H_{14}^+$ [80]. In a selection of studies on compact PAHs, the bare C_{24} carbon cluster emerges as the predominant component following complete dehydrogenation, while partially hydrogenated species $C_{24}H_x$ constitute minor components [see e.g. 80, 82, and references therein]. The variation in the reported photodissociation patterns is directly linked to the internal energy available. Ion trap experiments highlight a first route in which the initial phase involves a complete dehydrogenation. Calculations by Jone et al. [235] of possible isomers for the coronene skeleton C_{24} reveal that a closed cage fullerene and a bicyclic structure containing two rings of 14 and 10 carbon atoms, exhibit the highest thermodynamic stability. Once all hydrogen atoms are gone, further breakdown proceeds via elimination of C_2 and C_n units. This is consistent with the findings of Joblin et al. [81], who observed that C_{14}^+ dominates

the photodissociation mass spectra of the coronene cation (Fig. 3.35), using a cryogenic ion trap free from water vapor and H_2 contamination, and starting from the isotopically pure ^{12}C coronene precursor [81]. Under this scenario, the carbon cluster C_{11}^+ could be subsequently produced by the removal of C_3. This could be one of the reasons why C_{11} species dominate the final mass spectra of coronene dissociation experiments. Zhen et al. [236] also observed for dicoronylene ($C_{48}H_{20}$) the creation of clusters of C_n, where n>32, with a separation of two carbon atoms (i.e., C_{32}, C_{34}, C_{36}...). These large carbon clusters primarily originate from the loss of C_2 fragments from the large C_{42}.

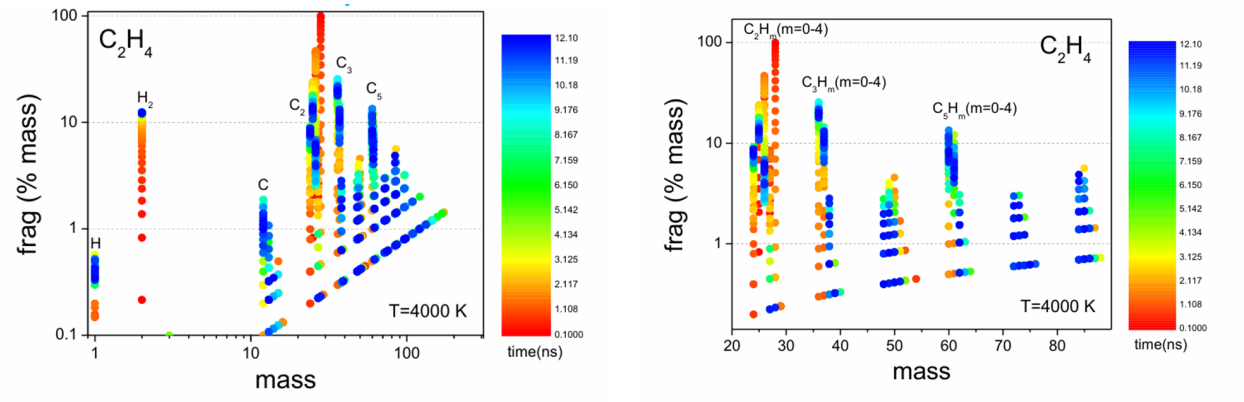
Other studies on coronene cation fragmentation reveal alternative dissociation pathways in which highly dehydrogenated species $C_{24}H_x^+$ are produced, suggesting that carbon fragments can be ejected before complete dehydrogenation. Such $C_{24}H_x$ formsafter sequential loss of -2H/H_2 atoms from the parent coronene molecule. (for eg. $C_{24}H_{10}$, $C_{24}H_8$, $C_{24}H_6$, $C_{24}H_4$ and $C_{24}H_2$.) Few examples of large clusters of coronene are mentioned below, where partially hydrogenated coronene $C_{24}H_4^+$ may form a variety of larger clusters. In the case of coronene, the $C_nH_x^+$ ions, where n=11–15, x=1–2 are the most commonly found fragments, like other similar PAH photodissociation experiments; n=11 is the most abundant carbon chain found in the high mass region of the spectra, and the majority of these are formed directly from the partially dehydrogenated coronene species. Hrodmarsson et al. [78] emphasized that their findings were consistent with previous photophysics research on PAHs; their work showed that C_n^+ (n=11–15) carbon clusters are the most likely fragments arising from the continuous irradiation of PAHs. The bare carbon cluster C_{11}^+ was recognized as a significant fragment subsequent to the total dehydrogenation of dicoronylene, similar to the findings for coronene [82]. Note that it is possible that these C_{11}^+ or C_{12}^+ chains could also be formed from the elimina-

tion of neutral C_3 from the C_{14}^+ and C_{15}^+ chains rather than directly from the parent molecules [237]. For corannulene too: C_{11}^+ carbon chains may also be synthesized directly from the parent corannulene cation, following two or more dehydrogenation steps, thereafter followed by ring opening and isomerization.

In order to acquire a deeper understanding of the mechanisms at play, the possibility of forming smaller hydrocarbons through a bottom-up process, starting from ethylene C_2H_4 (T=4000 K) was also investigated. The final distribution of clusters resembles that of coronene, with the formation of C_n and C_nH clusters with $n = 2, 3, 5$ and 7 in particular. Shocked ethylene tends to slightly favor the production of hydrogenated clusters C_nH with respect to coronene.

One of the key findings of OES complementary experiments is that the blackbody-like emission is also observed in the case of shocked ethylene as a precursor (Fig. 3.29). In order to acquire a deeper understanding of the mechanisms at play, the possibility of forming smaller hydrocarbons through a bottom-up process, starting from ethylene C_2H_4 (T=4000 K) was also investigated. The final distribution of clusters resembles that of coronene, with the formation of C_n and C_nH clusters with $n = 2, 3, 5$ and 7 in particular (fig. 3.42). Shocked ethylene tends to slightly favor the production of hydrogenated clusters C_nH with respect to coronene. The structureless character of this broad emission implies the spectral participation of a high number of isomers, as recalled earlier. Consequently, the higher end of the hydrocarbon distribution is expected to be the major contributor.

Our interpretation is that medium-size C_n clusters and C_nH_x hydrocarbons are formed behind the shock and are responsible for the blackbody-like emission. Cross-analysis suggests a distribution around 10 carbon atoms with odd-



(a) (b)

Figure 3.42: MD simulations of high-temperature processing of ethylene C_2H_4 (*a*); Presence of C_n and C_nH_x in ethylene (*b*) Mass 20-80: shows a large variety of C_nH_x clusters.*(Figures by Aude Simon).*

numbered species favored. These products may be formed via three possible pathways: by complete dehydrogenation and then fragmentation of the bare carbon cluster C_{24}, from the fragmentation of the partially hydrogenated clusters $C_{24}H_x$, but also from the recombination of hot fragments, in particular with C_2, C_2H and C_2H_2 according to MD simulations (Fig. 3.33). Reactivity with atomic H plays a small role, as its abundance slightly decreases with time. Some of the H radicals may end up in hydrogen gas. The formation of molecular hydrogen in the coronene experiments is comparable with the stable hydrocarbons observed in the post-shock analysis of the C_{60} with hydrogen experiments [115]. This suggests that hydrogen could be one of the gaseous end products resulting from coronene. The stable hydrocarbon products were identified using GC-MS and GC-FID; however, hydrogen cannot be detected with the current GC setup.

3.8.3 Small hydrocarbons and green emissions

Small hydrocarbons C_nH_x are considered good candidates for the broad emission which peaks at the wavelength of 540–550 nm. More specifically, this

component is attributed to the weakly hydrogenated C_nH_x hydrocarbon family, where n=3–7 and x=1–2 based on emission spectra obtained in prior investigations and MD simulations. Time-resolved measurements suggest that the carriers start to emit early, similarly to the blackbody-like emitters, with their abundance first rising, indicating a rise in concentration during shock processing, before the gradual decline in emission as the temperature decreases. It seems that the green emitters form early, and further fragmentation does not occur, indicating that these hydrocarbons are the final outcomes of fragmentation. Although the broad emission characteristics and the variety of smaller species, coupled with experimental high temperature and pressure conditions, limit the accurate assessment of the size of the emitters. We try to provide some constraints below.

Previous research on C_nH_x hydrocarbons with n<10 indicates that neutral species have low-energy linear geometries [238]. In the case of bare carbon clusters (x=0), odd-numbered C_n (such as C_3, C_5, C_7..) have cumulenic-type bonding, which is less reactive than the even-numbered polyyne-type structures (C_4, C_6, C_8). The degree of hydrogenation depends on the reactivity of the chains. According to Etem et al. [239], high-level ab initio quantum chemical calculations reveal that 60% of the 47 astronomically observed molecules consist of odd-numbered carbon chains, which demonstrate greater stability than even-numbered chains. The incorporation of hydrogen at both highly reactive terminals of polyyne-type chains leads to the generation of C_nH_2 clusters. In MD simulations, the formation of odd-numbered carbon clusters, C_3, C_5, and C_7, prevails over that of their even-numbered counterparts, C_4, C_6, and C_8, suggesting a reduced prevalence of small groups with an even number of carbon atoms (see Sec. 3.6). MD simulations for ethylene at 4000 K show a similar picture where the odd C_3H_x, C_5H_x, and C_7H_x, with x=0–4 domi-

nate the smaller hydrocarbon distribution, although the formation mechanisms of intermediate-mass species for PAHs and ethylene are fundamentally different, i.e., (mostly) top-down vs. bottom-up pathways. For the latter case, one can refer to pyrolysis studies in which molecular growth goes through a series of neutral reactions, including Hydrogen Abstraction–Acetylene Addition (HACA), Hydrogen Abstraction–Vinylacetylene Addition (HAVA), but also Phenyl Addition–DehydroCyclization, Radical-Radical Reactions, and Methylidyne Addition–Cyclization-Aromatization [52]. Chain elongation mechanisms involving C_nH and H lead to the formation of larger C_n and C_nH_x species in the case of shock-processing of ethylene.

Recent experiments can be very helpful to consolidate the *dehydrogenated small hydrocarbons* hypothesis. The study by Huo et al. [83] on soft X-ray photofragmentation of the coronene cation shows that $C_nH_x^+$ species dominate the mass spectra, with a major branching into $C_5H_x^+$, followed by $C_7H_x^+$ and $C_9H_x^+$. Studies on the collision of coronene with protons of energy in the 75–300 keV range also concur that $C_5H_x^+$ and $C_7H_x^+$ are the most abundant fragments in the low-mass region [91]. Investigation of keV collisions of multiply charged ions (He^{2+}, O^{3+}, and Xe^{20+}) with coronene and pyrene, highlights the formation of tiny C_nH_x units characteristic of linear-chain molecules [90].

L2MS measurements which analyze the molecular content of the post-shock solid residue show that only weakly hydrogenated carbon clusters C_nH_x (x=1–3) remain–as illustrated by the bottom left part of Fig. 3.34– with the exception of slightly altered leftovers of the initial material ($23 \leq n \leq 25$). The findings are consistent with previous observations, although L2MS probes the end products, which trace the entire process, including the rapid heating and cooling phases.

From all the above considerations, we can conjecture that the green emission observed in our experiments likely originates from C_nH_x hydrocarbons with n =3–9, odd-numbered n being more predominant, and with x=1–3.

3.8.4 C_3, C_2H and CH

The *C_3 radical*, which emits around 405 nm and has a similar oscillator strength as C_2, is not observed. This carbon species, which is expected to be formed in abundance during experiments, was absent as well in similar shock experiments conducted on fullerene processing and reported previously [3]. MD simulations hint at the presence of C_3, which becomes more dominant than C_2 at temperatures beyond 3500 K. The abundance of C_3 is attributed to the indirect formation of C_3 carbon chains through the dissociation of larger C_n or C_nH fragments. This hypothesis is supported by the experimental evidence mentioned here that the C_3 is an important fragment of the carbon chain dissociation, along with C_2. Experimental time-resolved spectra also indicate the absence of C_3 spectra.

The *C_2H small radical* appears crucial in the dynamics of the PAH dissociation process, as determined by the MD simulations conducted at temperatures ranging from 2500 to 4000 K. However, even if its expected broad characteristics, when combined with other underlying background features, complicate its identification, its signature remains undetected.

The *CH emission* in the UV-visible spectrum at 431 nm is briefly detected, consistent with MD calculations that suggest that a fraction of CH is produced at 4000 K. The recorded CH emissions in the experiments indicate the existence of CH fragments, either generated by the CH- loss pathway of smaller PAHs or recombination of C and H atoms ejected during the dissociation of coronene as

the MD simulations suggest that C and H atoms, along with the CH radicals are produced above 3500 K. Therefore, CH can be formed with atomic carbon and hydrogen recombination, which are available in plenty above 4000 K. Alternatively, the energetic considerations from DFT calculations demonstrate that, in comparison to H-loss, CH-loss is also a minor pathway. [82].

3.8.5 The road to nanostructures

Recorded pressure traces displayed with emission intensity profiles (Fig. 3.26) indicate that shock products are formed and remain at elevated temperatures, above 4000 K, for several milliseconds prior to condensation induced by the cooler expansion fan. The creation of carbon-rich, hydrogen-poor nanoparticles occurs during the cooling phase, as temperature and pressure decline from 4000 K and 30 bar to ambient conditions within ∼5–6 ms. The confined nature of the shocked region and the strong thermodynamic gradients play a critical role in the nucleation and growth of the solid phase, distinguishing this process from chemical vapor deposition, pyrolysis, or laser ablation methods.

As emphasised above, PAHs first undergo rapid dehydrogenation and fragmentation behind the shock, producing a variety of small hydrocarbons and carbon clusters. GC analysis confirm a pathway involving hydrogen loss and isomerization, forming reactive carbon units. The fragmentation is extensive under canonical ensemble conditions (thermalized, high-pressure), underscoring that continuous energy input via collisions is essential.

Although the details remain uncertain, the hot condensation sequence (above 2000 K) is likely driven by hydrogen abstraction - acetylene addition (HACA), and radical radical reactions (RRR) [52], which can build-up cycles and eventually evolve into more stable carbonaceous materials, displaying structural

features similar to those produced in gas-phase condensation experiments at temperatures in the 500–2000 K range. The L2MS mass spectrum provides molecular-level insight into the cooling phase, revealing bare carbon clusters and hydrogenated carbons, predominantly peri-condensed PAHs. A few products exhibit m/z values exceeding slightly that of coronene, indicating condensation and chemical growth processes. The absence of C_{60} in L2MS spectra suggests a multi-phase residue comprising intermediate-size carbon clusters that are easily desorbed, alongside more stable or embedded structures—such as nanometer-size particles or trapped fullerenes—that resist gas-phase detection.

XRD analysis of the post-shock residue reveals nanoscale carbonaceous particles with partial graphitic character. HRTEM imaging confirms the presence of diverse nanostructures—carbon nanotubes, nanoribbons, and carbon onions. Among these, polyhedral carbon onions dominate. They exhibit concentric graphitic layers with interlayer spacing of 0.35 nm, matching the (002) graphite plane, indicating a high degree of structural order.

According to prior studies on high-temperature soot transformation [240], the polyhedral morphology implies formation temperatures exceeding 2400 K, consistent with the elevated thermal conditions prevailing in the onset of the post-shock cooling phase. The formation pathways of these nanostructures share similarities with laser ablation methods, where a carbon-rich plume created by laser-induced vaporization of a graphite target cools and condenses into nanostructures. Graphene-like fragments generated in such plumes may either roll into nanotubes or curl into fullerenes via pentagonal defect formation. Further carbon accretion can lead to the development of carbon onions through self-assembly into concentric shells [58]. Likewise, high-temperature

laser pyrolysis of hydrocarbons such as C_2H_2, C_2H_4, and C_6H_6 has been shown to yield fullerene-like soot and nanostructures at temperatures above 3500 K [58]. In both cases, the process is marked by strong dehydrogenation.

In shock experiments, the sustained high density for milliseconds and the strong pressure gradient promote annealing and ordering, enhancing graphitic character and reducing structural defects. The addition of molecular hydrogen to the buffer gas does not alter the final products, indicating that hydrogen incorporation into the final structures is negligible.

3.9 Astrophysical implications

3.9.1 Shock-driven PAH dehydrogenation and hydrocarbon

Our study corroborates the view that coronene –and by extension other medium-sized PAHs– undergo strong dehydrogenation under shock conditions. This dehydrogenation process is accompanied by the formation of H_2 in contrast to the sequential atomic H loss observed in UV-driven PAH fragmentation [24, 75].

Molecular dynamics simulations, OES measurements and L2MS analysis show that shock processing at high velocities also efficiently produces a wide variety of carbonaceous fragments, including hydrogen-poor hydrocarbons and carbon clusters. For a given internal energy, strong resemblances with photodissociation studies are predicted. UV processing of small carbonaceous grains and PAHs has been proposed as a top-down mechanism explaining the observed concentrations of hydrocarbons, such as C_2H and c-C_3H_2, in the outer layers of photon-dominated regions exposed to low VUV flux [241, 242].

Astrochemical modeling by Awad et al. [243] confirmed that UV degradation efficiently produces small hydrocarbons such as CH, C_2H, and linear and cyclic isomers of C_3H_2 in diffuse clouds. It was concluded that both bottom-up and top-down mechanisms seemingly link simple hydrocarbons with PAHs in molecular clouds; nevertheless, the exact chemical pathways and their relative contributions remain unquantified [244].

Compared to UV-induced photoprocessing, shocks can deliver higher internal energies, often exceeding the fragmentation thresholds of PAHs. Ultraviolet photons responsible for photodissociation and photoionization in the interstellar medium typically range from a few eV to tens of eV, whereas low-velocity shock waves can impart energy to molecules from a few eV to several keV or more. High velocity shocks can even deposit energy in several 100 KeV. This should result in enhanced formation of C_nH_x species, which may contribute to observed interstellar hydrocarbon abundances.

The chemical environment in shocked regions further differs from that in UV-irradiated zones: high post-shock densities and temperatures promote subsequent gas-phase chemistry, including reactive collisions between carbonaceous products and association reactions with atomic hydrogen. As the gas cools behind the shock front, these conditions may favor the formation of larger carbonaceous molecules from smaller reactive fragments. This post-shock chemistry should play a key role in shaping the molecular inventory.

3.9.2 Shock-induced production of DIB carriers

The spectral analysis and interpretation presented in this work indicate that the family of small dehydrogenated hydrocarbons—as shock products of PAHs—are responsible for the broad green emission observed via optical emission spec-

troscopy (Sec. 3.8). However, determining their precise nature remains challenging given current experimental constraints. In our efforts to identify the green emitter(s), we found that the feature overlaps with a DIB centered at 5450 Å, observed in absorption (see figure 3.43 for comparison). Due to the high temperature and pressure conditions behind the laboratory shock wave—significantly different from those in the diffuse ISM—and the broad, continuum-superimposed nature of the emission, it is currently not possible to fully characterize this feature or draw direct comparisons with astronomical spectra. Nonetheless, examining proposed carriers of the λ5450 DIB remains instructive.

Linnartz et al. [4] first reported a spectral feature at 545.0 nm produced in an expanding acetylene plasma that matched both the central wavelength and width of the λ5450 DIB. Although they could not identify the carrier, they suggested it was a transient species composed of carbon and hydrogen. Later that year, gas-phase spectra obtained via cavity ringdown spectroscopy in a supersonic slit jet discharge with allene as a precursor led to the assignment of the band to the B^1B_1–X^1A_1 transition of H_2CCC [245]. However, the high column density required and the lack of additional spectral evidence in the ISM ruled out l-C_3H_2 as the sole carrier, though it may contribute in combination with other species at the same wavelength [246, 247, 48].

More recently, Marlton et al. [248] reported that the strongest visible band of $HC_{11}H^+$, with a central wavelength of 545.1 nm and a width of 1.5 nm, matches the λ5450 DIB. However, this identification remains unconfirmed, as other $HC_{11}H^+$ bands do not correspond to known DIBs, and the absence of smaller $HC_{2n+1}H^+$ chains complicates column density determinations.

A reliable identification of a DIB carrier requires a match in central wave-

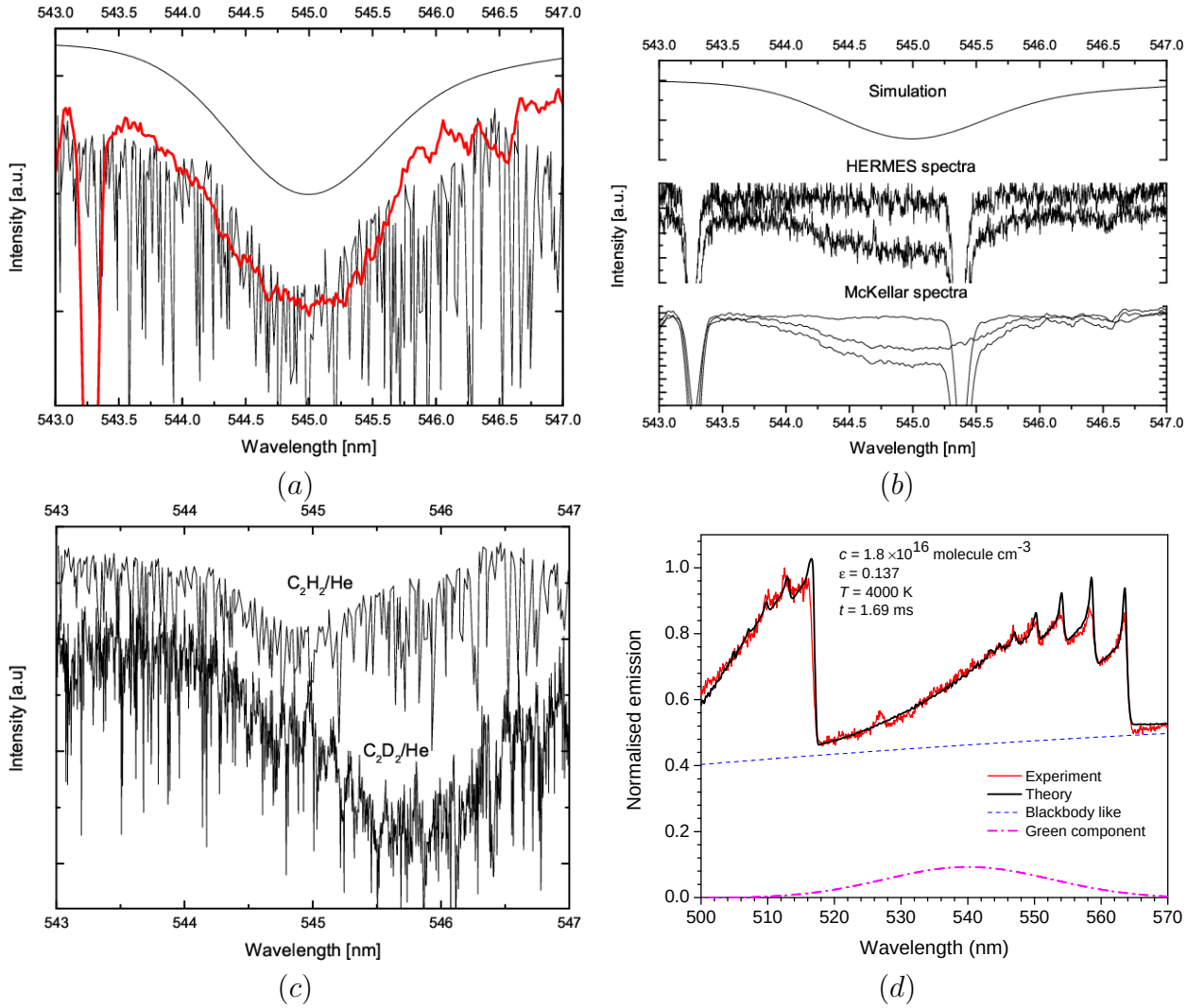


Figure 3.43: Comparison of laboratory spectrum and λ5450 DIB [4]: (a) The upper spectrum displays the digital λ5450 DIB, the middle spectrum presents the deblended McKellar data, and the lower spectrum illustrates the laboratory cavity ring-down absorption spectrum obtained from a supersonically expanding acetylene plasma. ; (b) The λ5450 diffuse interstellar band (DIB). The upper spectrum is a synthetic spectrum taken from DIB catalogs. The central and lower pictures display observational spectra obtained from the HERMES and McKellar spectrographs, respectively.; (c); Comparison of laboratory tests sampling expanding plasma utilizing ordinary acetylene (top) and deuterated acetylene (bottom) as precursor gases.(d) Coronene time-resolved spectra obtained at T_g= 4000 K. A similar broad green component is observed in corannulene, ethylene, and fullerene with H_2 (see figure 3.29).

length, width, and rotational profile across all vibrational bands in an electronic transition, as well as chemical plausibility, coverage of the DIB spectral range, and sufficient oscillator strength [48].

Given the contested nature of prior laboratory assignments, attributing the broad green component observed here to a specific species would be speculative. However, when combined with previous studies on carbon chains, molecular dynamics simulations, and results from complementary experiments (including L2MS analysis) (Sec. 3.8), small neutral dehydrogenated hydrocarbons of the form C_nH_x—with odd $n < 10$ and $x \leq 3$—emerge as plausible candidates.

3.9.3 Shock route to nanostructures

The current work, in particular through the L2MS analysis, suggests the formation of highly carbonaceous material from shocked PAHs. The formation of carbon nanotubes, ribbons, and onions, evidenced by HRTEM imaging, supports the scenario of fullerene-like conversion from (larger) PAHs in energetic environments such as interstellar clouds illuminated by strong UV radiation fields. The formation of fullerenes from the destruction of PAHs in space is considered to occur through a series of photochemical-driven processes that progressively break down and reorganize carbonaceous material. When large PAHs are exposed to intense UV radiation, particularly in PDRs and planetary nebulae, they undergo sequential dehydrogenation, where hydrogen atoms are stripped away, leading to more stable pure carbon structures [60]. They can then turn to graphene flakes, and restructure into more compact and curved forms, ultimately forming fullerenes such as C_{60} and C_{70} [76], which have been detected in planetary nebulae [249]. Depending on their energy, they can also

shrink by losing C_2 units, forming smaller rings and chains. The processes of dehydrogenation, isomerization, and skeleton shrinking are somewhat entangled and can take place simultaneously.

This study outlines a two-step route towards the formation of larger nanostructures, such as carbon nanotubes and carbon nano-onions. Laboratory experiments underscore a sequential process, resulting first from a top-down mechanism forming reactive carbon units, in particular small carbon clusters (heating phase), followed by bottom-up chemistry through nucleation of these clusters and reassembling into larger structures (cooling phase). Details of the second phase of such a process in space remain though elusive as carbon fragments will likely cool down before colliding with other carbon partners, through radiative emission or collision with more abundant atomic or molecular hydrogen. As a result, the energy of the products might not be high enough for the structure to easily reassemble or isomerize. This calls for further investigation.

However, carbon nanostructures could form in space directly through top-down processes. Recent shock-tube experiments indicate that shock processing of SiC dust analogues can yield various carbon allotropes such as graphite, graphene, carbon onions, and carbon nanotubes (Chandrasekaran et al., private communication). Similarly, slow thermal decomposition of SiC at 1300 K has been shown to produce fullerenes and nanotubes [250], supporting the idea that such nanostructures may form in circumstellar environments and be ejected into the interstellar medium during the planetary nebula phase. Once formed, these nanostructures are likely to be stable against UV radiation, potentially persisting over long timescales.

The detection of these nanostructures in space remains challenging due to their presumably low abundances. Nonetheless, some infrared emission features

observed in planetary nebulae—such as those at 6.6, 9.8, and 20 μm—have been tentatively linked to planar C_{24}, graphene precursors, or fullerenes [29]. Interstellar graphene may arise from photochemical processing of PAHs or fragmentation of graphite, with estimated abundances ranging from 5 to 20 ppm of C/H (about 2–7 % of total interstellar carbon) [251, 252].

Similarly, carbon nanotubes may form in the ISM via hydrogen abstraction and acetylene addition mechanisms, as suggested by DFT calculations [253]. Their interstellar abundance is constrained to a maximum of 10 ppm of C/H (around 4 % of total carbon) [254]. These species, including their hydrogenated and cationic variants, exhibit distinctive infrared vibrational features that might be detectable with instruments such as JWST.

3.10 Conclusions

In this chapter, the shock-induced processing of coronene $C_{24}H_{12}$, a prototypical compact PAH, was comprehensively investigated under laboratory conditions sharing some of the characteristics found in energetic astrophysical environments. Using a pressure-driven shock tube, the shock processing of PAH, fullerene, and hydrocarbons was studied using various techniques, including *in situ* optical emission spectroscopy and *ex situ* analysis of solid residues. To study time-resolved emission spectroscopy, we developed a home-built broadband emission spectrometer with high resolution and sensitivity. The investigations focused on PAH, supplemented with complementary experiments involving fullerene and ethylene. The findings have been confirmed through MD simulations and *ex situ* analysis of solid residues conducted by various collaborators. The ex situ analysis of solid residues comprises infrared

spectroscopy, Raman spectroscopy, L2MS, XRD, and TEM, revealing the key pathways in the transformation of PAHs under shock conditions.

Our findings reveal a dominant dehydrogenation pathway for coronene upon exposure to temperatures reaching 4000 K. This process leads to the formation of molecular hydrogen and a diverse range of carbonaceous products. *In situ* realtime spectroscopy confirms the presence of C_2 radicals as a major gas-phase component, alongside a broad continuum emission attributed to both large carbon clusters C_n and medium-size hydrogen-poor hydrocarbons C_nH_x. These results call for a more quantitative analysis of the volatile shock products through, e.g., online mass spectrometry measurements connected to the shock tube.

Ex situ analysis of solid residues demonstrates the formation of graphenic/graphitic nanostructures, including carbon nano-onions, nanotubes, and nanoribbons, suggesting a sequential pathway from PAHs to more complex carbonaceous materials. PAHs first lose hydrogen and are broken down into smaller reactive carbon units just behind the shock, before reassembling into larger structures when the gas cools. The L2MS analysis validates carbonization of the shock products. Our results suggest that shocks could contribute to the formation of nanostructures in space in their wake.

Molecular dynamics simulations corroborate most of the experimental observations, highlighting the importance of dehydrogenation and fragmentation in the initial stages of coronene breakdown. The simulations further suggest the formation of key intermediate species, such as C_2 and small carbon clusters and hydrocarbons, and provide insights into the kinetic rate of the dissociation process. The absence of detectable C_3 emission, despite its predicted formation in MD simulations, points to the potential role of collisional quenching or

conversion into a long lifetime triplet state.

These results contribute to the understanding of the lifecycle of carbon in the interstellar medium. Shock waves, prevalent in diverse astrophysical environments, can drive the transformation of PAHs into smaller hydrocarbons and graphene flakes. These processes contribute to the overall carbon budget of the ISM and might play a role in the formation of some DIB carriers. The identification of C_nH_x species as potential carriers of the broad green emission observed in our experiments requires further investigation regarding a potential link to the λ5450 DIB.

This study in particular underscores the value of shock tubes as a crucial tool in laboratory astrophysics, enabling the controlled reproduction of the high temperatures and energy inputs characteristic of astrophysical shocks. A central feature of the process observed here is its sequential nature: an initial top-down phase, in which fast heated PAHs undergo dehydrogenation and fragmentation into smaller units, is followed by a bottom-up reassembly of shock products into larger, nanometer-scale carbonaceous structures. In contrast, smaller hydrocarbons such as ethylene utilize a bottom-up approach to produce similar nanostructures. The primary link between the top-down and bottom-up pathways is the extensive green emission feature due to the C_nH_x species, correlated with the λ5450 DIB feature observed in both experiments.

Bottom-up and top-down mechanisms connect simple hydrocarbons with polycyclic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM), also. However, the specific chemical pathways and their contributions remain unclear. Shock tube studies offer insight into the relationship between top-down and bottom-up pathways. While this staged evolution may not fully capture the complexity of astrophysical environments—where such processes may

overlap or compete—it nonetheless provides critical insights into the chemical pathways that govern PAH transformation. By combining *in situ* diagnostics with *ex situ* analysis, this approach enables a comprehensive investigation of the formation and destruction mechanisms of key species in the ISM, shedding light on the lifecycle of complex carbonaceous materials under extreme conditions.

This work provides a framework for future studies aimed at unraveling the complex interplay between PAHs, shocks, and the evolution of carbonaceous materials in space.

Chapter 4

Unimolecular decomposition of hydrindane

Abstract of the chapter

Bicyclic alkanes are considered key components of various fuels, including aviation and diesel fuel. Trans-hydrindane (HYD) (C_9H_{16}) is an ortho-fused bicyclic hydrocarbon consisting of a six-membered ring fused to a five-membered ring. The chemical properties are particularly analogous to trans-decalin (C_9H_{18}), the most frequently used bicyclic alkane surrogate. Evidence for their presence in the fuels is well documented; nevertheless, the mechanism of pyrolysis of HYD has never been studied. This work aims to investigate the thermal decomposition of HYD, a prototypical bicyclic alkane, identify the gaseous products formed, and develop a pyrolysis mechanism.

The thermal decomposition of trans-hydrindane (HYD) at elevated temperatures in an argon bath gas was conducted using a single-pulse chemical shock tube (CST-1) facility in our laboratory. Experiments were conducted within a temperature range of 1000-1550 K and a corresponding pressure range of 12.8-23.3 bar, with a dwell time of 1.40-1.54 ms. The post-shock products were

analyzed using gas chromatography coupled with flame ionization detection and mass spectroscopy.

The unimolecular decomposition of hydrindane has been investigated using the CASSCF/MRCI (multireference) and B3LYP/CBS-QB3 (single-reference) methods. Geometry optimization and vibrational frequency calculations were performed for reactants, transition states, and products using the CASSCF method with the 6-31+g(d,p) basis set and the B3LYP method with the 6–311G(2d,d,p) basis set. The single-point energies were calculated via the MRCI and CBS-QB3 methods. This chapter explores various steps of hydrindane dissociation. Unimolecular dissociation leads to the generation of the hydrindane radical by the loss of an H radical, ring-opening isomerization to olefinic intermediates, formation of the hydrindane radical via H-abstraction, and the decomposition and isomerization of hydrindane radicals. The high-pressure limit (HPL) rate constants are calculated using variational transition state theory (VTST) and conventional transition state theory (TST) within the temperature range of 800–2000 K. The thermal rate constants for reactions without a saddle point are calculated utilizing VTST, and the remaining reactions, which are determined by a single saddle point transition state, are obtained using TST. The initial unimolecular decomposition reaction of cycloalkanes represents a crucial step in the pyrolysis and oxidation processes of all cycloalkanes. Hence, the unimolecular decomposition and ring-opening isomerization energy barriers and thermal rate constants were compared with prior theoretical studies involving monocyclic alkanes (cyclohexane, cyclopentane) and bicyclic alkanes (decalin). This work aims to provide a comprehensive description of the thermal decomposition using quantum chemistry methods and to develop a detailed chemical kinetic model for investigating the pyrolysis of hydrindane in shock tubes. A detailed kinetic model comprising 484

species and 1774 reactions was developed using computational calculations and existing models to simulate the experimental data observed.

A range of pyrolysis products was identified and quantified, with particular importance on abundant products such as methane, ethylene, acetylene, and cyclic C6- and C7-intermediates (including benzene, 1,3-cyclohexadiene, cyclohexene, and toluene, among others). The rate of production (ROP) and sensitivity analysis of HYD under pyrolysis conditions have been investigated, with an emphasis on the unimolecular dissociation/initial decomposition stages of HYD, as well as the formation of benzene derived from kinetic simulations. From the reaction pathway analysis, we conclude that the decomposition of HYD originates with C–C bond dissociation; however, H-atom abstraction processes are most important for the consumption of HYD. The pyrolysis conditions that result in aromatics, such as benzene, styrene, and toluene, require the presence of resonance-stabilized radicals, including allyl, propargyl, butadienyl, phenyl, and benzyl radicals. Finally, the overall rate constant for the decomposition of HYD was calculated to be

$$k(s^{-1}) = 10^{8.1\pm0.25} exp \frac{(-34.6 \pm 1.5) kcal/mol}{RT}$$

4.1 Background

Trans-hydrindane (HYD) may be selected as a surrogate component for analyzing transportation fuel, comparable to trans-decalin, as previously mentioned. Consequently, HYD has been investigated in this chapter. Figure 4.1 shows the scheme for the initial decomposition channels of HYD: unimolecular decomposition and ring-opening isomerization of HYD. The decomposition of hydrindane can proceed via two possible pathways: a unimolecular reaction

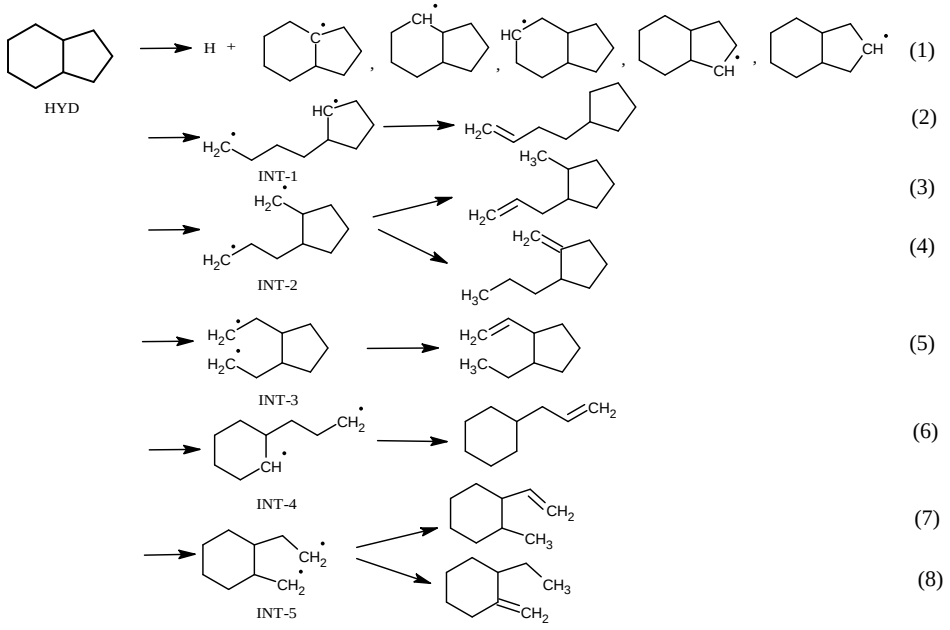


Figure 4.1: Scheme for the unimolecular decomposition and ring-opening isomerization of hydrindane.

involving the dissociation of a C-H bond or through ring-opening isomerization. Isomerization takes place via a two-step mechanism. The CP or CH ring first experiences C-C bond dissociation, leading to the generation of biradical intermediates. In the next stage, H-migration occurs, resulting in the formation of alkenes. The competition between ring-opening isomerization and C-H bond dissociation pathways determines the major pathways of the initial routes of HYD consumption.

To address the lack of literature on the theoretical and experimental decomposition of hydrindane, we present the first investigation into the thermal decomposition of HYD using shock tube pyrolysis, computational analysis, and kinetic modeling. The study includes:

1. The pyrolysis experiment of HYD was performed in a single-pulse shock tube (CST facility) at elevated pressure and temperature conditions (specify T and P). GC-FID/FID and GC-MS have been employed for the detection, identification, and quantification of the detected products.

2. This work also conducts a detailed investigation of the chemical pathways involved in HYD pyrolysis using quantum chemistry methods, incorporating single-reference and multireference calculations as necessary. This study provides a detailed description of unimolecular dissociation (loss of the -H) and ring isomerization pathways of HYD, H-abstraction reactions, and isomerization and decomposition of HYD radicals utilizing high-level ab initio calculations. The reaction rates were determined based on the calculated potential energy surfaces using transition state theory (TST) and variational transition state theory (VTST) across a wide temperature range of 800-2000 K.

3. Finally, a detailed chemical kinetic model for HYD pyrolysis was established, identifying the rate constants of significant initial reactions using advanced quantum calculation methods. The newly developed model was validated using experimental measurements of HYD pyrolysis. The ROP and sensitivity analysis of HYD under pyrolysis conditions have been investigated, with an emphasis on the unimolecular dissociation/initial decomposition stages of HYD, as well as the formation of toluene and benzene derived from kinetic simulations.

This thesis chapter is structured in the following manner: Section 4.2 describes the experimental methods used to investigate the thermal decomposition of hydrindane. Section 4.3 describes the computational methodology used to investigate the thermal decomposition of hydrindane. The section includes details of the quantum chemistry methods used for geometry optimization, frequency calculations, and reaction rate calculations. The results of the theoretical calculations are discussed in Section 4.4. The section includes the potential energy surface diagrams and considers the reaction mechanisms involved. Fur-

thermore, the high-pressure limit (HPL) rate constants computed based on quantum chemistry calculations for the temperature range of 800–2000 K are discussed. Section 4.5 discusses the pyrolysis experiments and kinetic simulations. The identified chemical routes from GC results are employed in ANSYS Chemkin, and the resultant products are simulated throughout a temperature range of 1000K to 1550K for comparison with experimental data on HYD pyrolysis. This section also analyzes the ROP and sensitivity of HYD during pyrolysis conditions. Section 4.6 is the conclusion part of our study.

4.2 Experimental methods

The thermal decomposition of HYD was studied in the Chemical Shock Tube facility (CST-1). The specifications of the shock tube equipment are as follows. This section outlines some essential features. This section gives some essential features. The CST comprises an aluminum tube with an internal diameter of 50 mm and a wall thickness of 25 mm. The length of the driver section is 1.8 m, and that of the driven section side is 3.3 m. The manual ball valve is positioned in the driven section, 0.4 m from the end flange, and the region between them is referred to as the sample chamber, also known as the reaction chamber. Although this method was introduced by Tschuikow-Roux et al. in 1970 [189], it has recently been referred to as the constrained reaction volume strategy by Hanson's group [255]. The experiment utilized an aluminum diaphragm with a thickness of 1-2 mm and variable grooving for bursting.

Axially mounted PCB pressure transducers (model 113B22, with a sensitivity of 1 mV/psi, and model 113B24, with a sensitivity of 5 mV/psi) were used to measure pressure signals at distances of 5 mm and 85 mm from the endwall of the driven section. The time intervals between the rising fronts of

the pressure trace from the incident shock are utilized to calculate the incident shock velocity and Mach number. The actual T_5 temperature has been calculated with a correlation between T_5(theoretical) and T_5(kin) using an external chemical thermometry method. The T_5 (theoretical) temperature behind the reflected shock waves was calculated from the incident shock velocity using the standard one-dimensional normal shock equations from the Wisconsin Gas Dynamics Calculator [256]. T_5 (kin) was determined utilizing the previously known rate constants of ethyl chloride and 1,1,1-trifluoroethane as external chemical thermometers within the temperature ranges of 960–1300 K and 1300–1500 K, respectively, as described in earlier studies. [185, 257].

A mixture of HYD (3 mmHg vapor pressure at 25°C) ($\geq$ 98% purity, TCI (Tokyo Chemical Industry)) and argon (99.999% purity) was generated by diluting the sample in argon gas. The Edward (TCI pumping station) and Adixen (ATP 400) turbomolecular vacuum pump systems have been used to evacuate the driven and driver sections up to 10^{-6} mbar. The sample chamber has been maintained at a temperature of 343 K throughout the experiments to prevent the formation of liquid droplets from the sample and its resulting substances. The freeze-pump-thaw technique is used to eliminate any dissolved volatiles and air before the sample injection. We utilized a mole fraction of 0.0006–0.0008 of the HYD in argon for the study. The quantification and identification of the pre-shock and post-shock gas mixtures were performed utilizing a gas chromatograph with a dual flame ionization detector (GC-FID/FID, Agilent 7890B) and a gas chromatograph coupled with a quadrupole mass detector (GC-MS, Agilent 7890A). The flame ionization detectors of the gas chromatograph have been calibrated with hydrocarbons, utilizing known quantities of reference gases. The calibration procedure has yielded an estimated error of 5%.

4.3 Computational methods

4.3.1 Quantum chemistry calculations

Ab initio methods were employed to determine all the stationary points, including the ground state, transition state, and products. These results were then utilized in the transition state theory (TST) calculation to ascertain the kinetics of the unimolecular decomposition processes. CASSCF/MRCI (multireference) [192] and CBS-QB3 (single reference) [193] approaches have been utilized for the computations. The stationary points were confirmed using a harmonic vibrational analysis and were classified as either a minimum or a transition state based on the presence of one imaginary frequency along the reaction coordinate. The number of imaginary frequencies dictates the nature of the stationary point in the geometry: 0 for a structure that is a local or global minimum in the potential energy hypersurface and 1 for a transition state. According to the standard transition state theory, the saddle point in a reaction is considered the bottleneck since it has the most electronic energy. Intrinsic Reaction Coordinate (IRC) calculations are performed in both directions (reactant and product), beginning with the optimized transition state structure, and the saddle point is confirmed to ensure that the saddle point connects the right reactant(s) and product(s).

As depicted in the Figure 4.1 , for the unstable biradical intermediates involved in the ring-opening isomerization and the unimolecular decomposition reaction (elongated C-C and C-H bond lengths during the bond dissociation reaction) utilize multireference calculations calculations were carried out. The multireference configuration interaction (MRCI) method integrates the multiconfiguration self-consistent field (MCSCF) approach, with the complete ac-

tive space self-consistent field (CASSCF) being the most commonly utilized method, alongside traditional configuration interaction (CI) techniques. The geometry optimizations and frequency calculations were performed utilizing the CASSCF (complete active space self-consistent field) (zero-point energy (ZPE) scaling factor is 0.932) method with the 6-31+g(d,p) basis set. For the C-H, C-C bond dissociation, and biradical intermediates, the minimum active space of two electrons occupying two orbitals (i.e., CAS(2e,2o)) is considered. HYD comprises 35 doubly occupied molecular orbitals. Thus, the active orbitals in CAS (2e, 2o) correspond to orbital numbers 35-36. Corrections to single-point energies have been performed using the MRCI approach with a similar active space and basis set. The CBS-QB3 method was employed to compute the H-abstraction and HYD radical decomposition processes, and so on. In the first step, the geometry optimization and frequency calculations were conducted using the B3LYP (Becke 3-parameter Lee-Yang-Parr) [194] hybrid density functional method with the 6–311G(2d,d,p) basis set (zero-point energy (ZPE) scaling factor of 0.99). The second step involves complete basis set extrapolation to correct the total energy. Multireference computations were conducted using the Molpro 18 and 24 quantum chemistry software [258, 196]. The remaining single-reference computations were conducted using the Gaussian 16 program.

4.3.2 Reaction rate constant calculations

High-pressure limit thermal rate constants for all the elementary reactions of HYD associated with a saddle point (transition state) were calculated utilizing

conventional transition state theory (TST).

$$k(T) = \sigma \frac{k_B T}{h} \frac{Q_{\neq}}{\Pi Q_R} exp(-\frac{\Delta E_0}{RT})$$

where σ is the symmetry number, k_B is the Boltzmann constant, h is the Planck's constant, T is the temperature, Q_R is the total molar partition function for reactants (consisting of the translation, vibration, and rotation), $Q_{\neq}$ is the partition function of the activated complex, and ΔE_0 is the electronic energy barrier, including ZPE. To compute the activation energy barrier (ΔE_0), the reaction path has been defined as the path with a minimum energy along the potential energy surface that links the reactants and products while traversing the transition state. The C-H bond dissociation channel is a barrierless reaction requiring a variational treatment. The transition state's position relative to the temperature was ascertained by a variational method by minimizing the rate constant as a function of reaction coordinate(s) at temperature (T) within the specified temperature range (800-2000 K).

$$k_{VTST} = min k_{TST}(s, T)$$

where $k_{TST}(s, T)$ represents the rate constant at each location along the reaction coordinate.

To implement chemical kinetic modeling effectively, three kinetic parameters, A, n, and, E_A are determined by fitting the calculated rate constants across a temperature range of 800-2000 K in increments of 50 K to a modified Arrhenius equation. The kinetic parameters A, n, and, E_A are ascertained by fitting the computed rate constants throughout a temperature range of 800-2000 K in 50 K intervals to a modified Arrhenius equation. Considering the reasonable correlation obtained with the temperature coefficient, which yielded

a value of n = 0 within the studied temperature range, we decided to maintain the temperature coefficient at zero and used the standard Arrhenius equation shown below:

$$k(T) = Aexp(-\frac{\Delta E_a}{RT})$$

The calculations of the rate constants were performed utilizing the Multiwell 2023 program package [198, 199, 200]. The thermal module of the multiwell allowed conventional transition-state theory (TST) calculations, while the ktools module was employed for variational transition-state theory (VTST) calculations. Partition functions were calculated using the vibrational frequencies and rotational constants obtained from the quantum chemistry calculations mentioned in the previous section. The restricted rotations of the cyclic structure were additionally considered harmonic oscillators, incorporating the flexible movements of the ring. This study excluded the quantum tunneling effect because of the comparatively low barriers associated with reactions involving H atoms, such as H-abstraction and H-migration, and the high temperatures investigated.

4.4 Results and Discussion

The initial steps of the thermal decomposition of HYD and the subsequent reactions can be organized into various stages.

1. Unimolecular decomposition and ring-opening isomerization of HYD: The reaction involves the dissociation of the C-H and C-C bonds, resulting in the formation of HYD radicals and biradical intermediates. Following this, the subsequent step yields seven alkenes through five distinct biradical intermediates.

2. H-abstraction reaction of HYD by H atom and CH_3 radical: The chain reactions occur through H-abstraction from five distinct carbon centers of HYD by an H atom and a methyl radical. The H-abstraction results in five different types of HYD radicals.

3. Dissociation and isomerization of hydrindane radicals: HYD radicals can either isomerize (ring-opening) to form cyclic alkenyl radicals or yield cyclic intermediates by sequential dehydrogenation. Secondary reactions can occur via the decomposition of such alkenes and alkenyl radicals.

4. Decomposition and isomerization of alkenyl cyclohexane and cyclopentane radicals: The alkenyl cyclohexane and cyclopentane radical decomposition reactions are further taken from cyclopentane and cyclohexane submechanisms, respectively.

In the following discussion, we consider the potential energy surface (PES) diagram of HYD decomposition, including the reaction channels for all previously mentioned reactions. Subsequent to the PES section, this discussion will focus on the high-pressure limit (HPL) thermal rate constants relevant to each reaction.

Our calculations begin with the lowest energy conformer of trans-hydrindane, as determined by CBS-QB3 calculations.

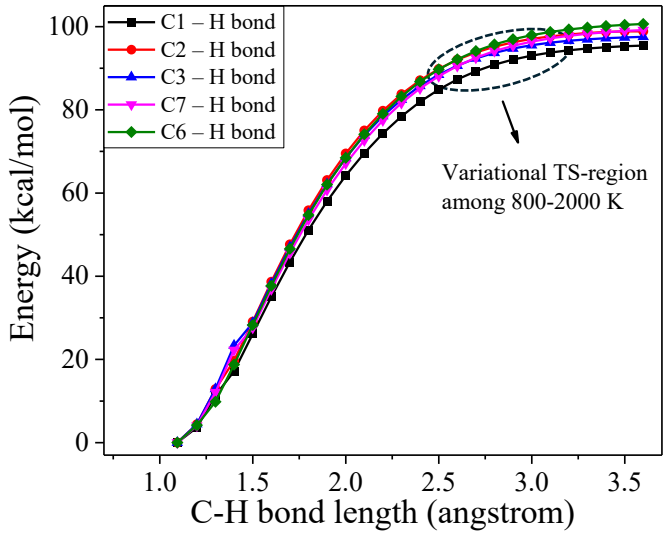


Figure 4.2: Stepwise optimized potential energy curve of C-H dissociation of HYD at MRCI/6-31+g(d,p)//CAS(2,2)/6-31+g(d,p) Energy unit: kcal/mol.

4.4.1 Unimolecular decomposition and ring-opening isomerization of hydrindane

Figure 4.1 illustrates all potential reaction pathways for the initial unimolecular dissociation and ring-opening isomerization routes of HYD. In the first step, five HYD radical intermediates are formed via C-H bond dissociation. In the second ring-opening step (C-C bond dissociation), seven different olefinic intermediates are formed via five different biradical intermediates. C-H and C-C bond dissociation channels are examples of bond fission reactions. Such reactions show significant multireference characteristics as the chemical bond is stretched. The decomposition pathways of C-H bond dissociation (i.e., reaction 2) and C-C bond dissociation (i.e., reactions 2-8) are calculated with the CASSCF//MRCI method, which involves two active space orbitals that correspond to the C-C bonding orbital and the C-C antibonding orbital. The C-H dissociation channel has no saddle point along the reaction coordinate. The

minimum energy potentials (MEPs) for C-H were determined by performing a relaxed scan along the reaction coordinates with a step size of 0.1 Å via the MRCI//CASSCF method (Figure 4.2).

Figure 4.3 shows the potential energy surfaces of all the possible reaction pathways shown in Figure 4.1. The calculations for unimolecular dissociation and ring-opening isomerization were performed at the MRCI//CAS(2,2)/6–31+g(d,p) (red color) and CAS(2,2)/6–31+g(d,p) (black color) level of theory. The C-H BDE depends on the position of the carbon atom (secondary or tertiary), and the C-C BDE depends on the type of ring (CP or CH) and the position of the C-C bond relative to the tertiary carbon center. The PES shows that the unimolecular dissociation channels have a higher energy barrier than the ring-opening isomerization step. The C-H bond dissociation occurs at five distinct carbon atoms (C1-H, C2-H, C3-H, C7-H, and C8-H). The BDE at the tertiary carbon atom (C1-H), leading to a more stable tertiary radical, is the lowest in the case of HYD.

Ring-opening isomerization of HYD occurs in two steps. Initially, the HYD undergoes C–C bond dissociation, resulting in the formation of biradical intermediates. HYD has five unique C-C ring bonds: the cyclopentane ring (C6-C7 and C7-C8) and the cyclohexane ring (C1-C2, C2-C3, and C3-C4). The dissociation by ring-opening can produce a total of five biradical intermediates, including the CP ring (biradical INT4 and biradical INT5) and the CH ring (biradical INT1, biradical INT2, and biradical INT3). The ring opening of the 5-membered ring has a lower energy barrier, with the formation of INT1 (C6-C7, adjacent to the tertiary carbon atom) being the lowest. Similarly, in the ring opening of the 6-membered ring, the lowest BDE is of the C-C bond (C1-C2) adjacent to the tertiary carbon atom. Table 4.1 shows the compari-

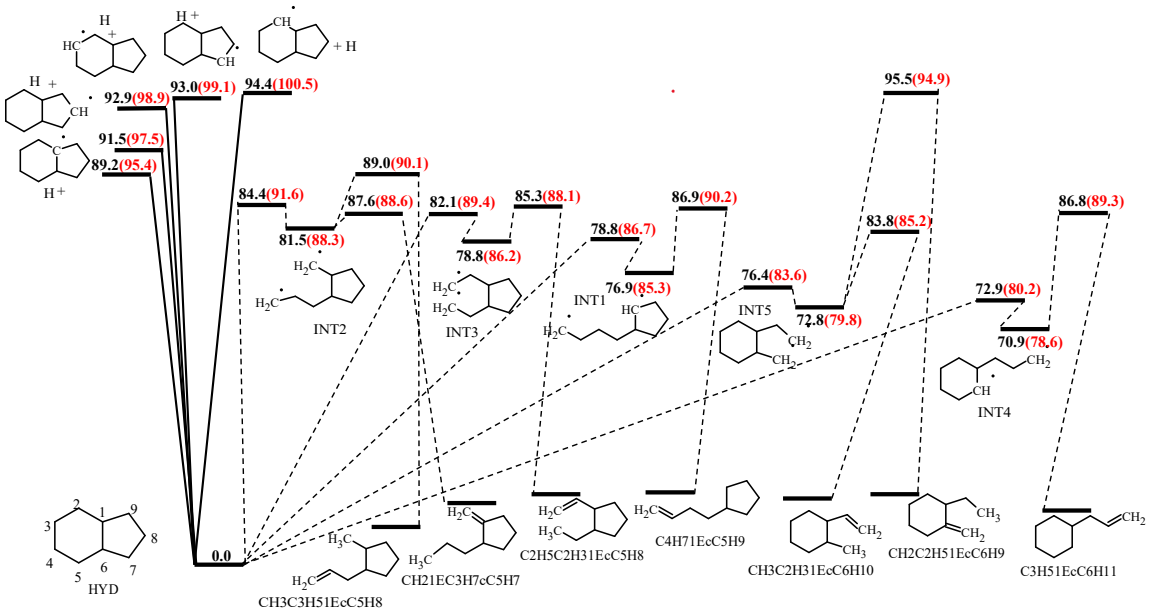


Figure 4.3: Potential energy surface for unimolecular decomposition (C1-H, C2-H, C3-H, C7-H, and C8-H bond dissociation) and ring-opening isomerization (ring C1-C2, C2-C3, C3-C4, C6-C7, and C7-C8 bond dissociation) of hydrindane. Methods were MRCI/6-31+g(d,p)//CAS(2,2)/ 6-31+g(d,p) (value in the bracket with red color) and CAS(2,2)/6-31+g(d,p) (value with black color). Energy unit: kcal/mol.

son of the TS barrier of the unimolecular decomposition (C-H bond scission) and the first step of the ring isomerization channels (formation of biradical intermediates via C-C bond scission) of cyclohexane, cyclopentane, hydrindane, and decalin. The table indicates that the ring-opening step is the most favorable reaction channel in all the cycloalkanes (C-H BDE is more than 10 kcal/mol than that of C-C BDE). Similar to HYD in decalin, too, the BDE at the tertiary carbon atom (C1-H) and the C1-C2 bond (adjacent to the tertiary carbon atom) are the lowest. The bicyclic alkanes will dissociate faster than their parent cycloalkanes (for example, HYD will dissociate faster than CP and CH, whereas decalin will dissociate faster than CH). [259] In the second step, the biradicals undergo intramolecular H-migration, in which a radical abstracts a hydrogen atom from a carbon atom adjacent to the second radical. These reactions result in the formation of seven alkene isomers. Intramolecular H-

Table 4.1: Comparison of the relative energy barrier of the unimolecular decomposition (C-H scission) and ring-opening step of isomerization (C-C scission) of cyclohexane, cyclopentane, hydrindane, and decalin. Method: MRCI Energy unit: kcal/mol.

	CH[a]	**CP**[b]	**HYD**[c]	**decalin**[d]
Unimolecular decomposition (C-H dissociation)				
TS of C1-H	97.8	97.5	95.4	97.0
TS of C2-H	-	-	100.5	102.4
TS of C3-H	-	-	98.9	99.9
TS of C7-H	-	-	99.1	-
TS of C8-H	-	-	97.5	-
Ring-opening isomerization (C-C dissociation)				
TS of C1-C2	88.7	85.9	86.7	85.4
TS of C2-C3	-	-	91.6	84.0
TS of C3-C4	-	-	89.4	86.9
TS of C6-C7	-	-	80.2	-
TS of C7-C8	-	-	83.6	-

[a] CASPT2/cc-pVDZ [259] ; [b] MRCI (This work); [c] MRCI (This work); [d] MRCI [130].

migration energy barriers depend on six- or five-membered cyclic transition states (depending on the CH or CP ring of hydrindane). A six-membered cyclic transition state is more favorable than a five-membered one because of the reduced ring strain. This allows for a more relaxed geometry and a lower energy barrier during the transition state, which increases the probability of the reaction proceeding via a six-membered transition. In this cyclic TS state, the barriers are again dependent on whether the H transfer takes place from the carbon chain to the CP or CH ring or vice versa, and the H transfer from one carbon chain to another carbon chain. An H transfer from one carbon chain to another carbon chain will have the lowest energy barrier in both the cyclic TS states. The H transfer from the ring to the carbon chain or vice versa will also have comparatively higher energy barriers than the H transfer from one carbon chain to another carbon chain. Table 4.2 shows the details of the different cases of H migration in the second step of ring opening of hydrindane and decalin (only a six-member cyclic transition is possible). INT1 (H transfer from carbon chain to CP ring) in the 6-membered transition for both HYD and decalin has the highest energy barrier. Biradicals INT1, INT2,

Table 4.2: H-migration TS energy barriers. Methods: CAS(2,2)/6-31+g(d,p) Energy unit: kcal/mol.

H-migration details	**HYD**	**decalin**
Six-membered cyclic TS states.		
INT1 = C4H71EcC5H9 (H-transfer from carbon chain to CP ring)	10.1	7.1
INT2 = CH3C3H51EcC5H8 (H-transfer from carbon chain to carbon chain)	6.5	4.5
INT2 = CH21EC3H7cC5H7 (H-transfer from CP ring to carbon chain)	6.1	-
INT3 = C2H5C2H31EcC5H8 (H-transfer from carbon to carbon chain)	7.5	4.6
Five-membered cyclic TS states		
INT4 = C3H51EcC6H11 (H-transfer from carbon chain to CH ring)	15.9	-
INT5 = CH3C2H31EcC6H10 (H-transfer from the carbon to carbon chain)	11.0	-
INT5 = CH2C2H51EcC6H9 (H-transfer from the CH ring to carbon chain)	22.6	-

and INT3 (six-membered cyclic TS states) have lower energy barriers than INT4 and INT5 (five-membered cyclic transition states). H transfer reactions from one carbon chain to another carbon chain, in the case of 5-membered (INT5 = CH3C2H31EcC6H10) and 6-membered (INT2 = CH3C3H52EC5H8 and INT3), have lower energy barriers. The H transfer reaction from a carbon chain to a ring in cases of 5-membered (INT5 = CH2C2H5) and 6-membered (INT = C4H7) has the highest energy barriers. INT5 = CH2C2H51EcC6H9 (H transfer from the ring to the carbon chain) has the highest energy barrier for the 5-membered cyclic TS due to the H transfer from the CH ring to the carbon chain.

4.4.2 H-abstraction reaction of HYD by H atom and CH_3 radical

An essential reaction in combustion includes the removal of an H-atom by radicals such as OH, H, HO_2, O, and CH_3 reacting with a molecule. In the absence of oxygen for the pyrolysis reaction, we consider only H and CH_3 abstraction. The CBS-QB3 level of theory was used for all the abstraction reactions. Geometry optimization and vibrational frequency computations were carried out at the B3LYP/6-311G(2d,d,p) level. Figure 4.4, 4.5 shows the potential energy surface for all the possible H-abstraction reactions. Hydrindane possesses five

Table 4.3: Comparison of the energy barrier of the H-abstraction reaction by H atom and CH_3 radical between hydrindane and decalin. Energy unit: kcal/mol. Method: CBS-QB3

Description	**HYD (H, CH_3)**	**decalin (H, CH_3)**
C1 (H) abstraction T1X	4.4, 8.3	4.9, 8.7
C2 (H) abstraction S2X	7.6, 11.4	7.3, 11.0
C3 (H) abstraction S3X	7.4, 11.1	7.5, 11.3
C7 (H) abstraction S7X	7.4, 11.2	-
C8 (H) abstraction S8X	6.4, 10.4	-

distinct carbon atom sites (T1X, S2X, S3X, S7X, S8X) for hydrogen removal by hydrogen or methyl radicals. These reactions proceed via the cleavage of the existing (C-H) bond in the presence of radicals and the production of new (stronger H-H, C-H) bonds. The positions of hydrogen atoms (primary, secondary, and tertiary) and the C-H BDEs significantly influence hydrogen abstraction. When CH_3 radical and H atom abstract a hydrogen atom from the molecule, it can lead to the formation of CH_4 (methane) and H_2 (hydrogen), respectively. Table 4.3 compares the H-abstraction of HYD and decalin. The PES and the table for H-abstraction also show the energy barrier for carbon andcondary carbon $>$ tertiary carbon in both HYD and decalin radicals. The energy threshold for hydrogen abstraction by an H atom is less than that for a methyl radical. H radicals show greater reactivity than the alkyl or allyl radicals tend to, as these can be stabilized by hyperconjugation and inductive processes; hydrogen radicals lack any such stabilization. H abstraction at the tertiary position (C1-H) has the lowest energy barrier for H abstraction. The C1-H bond (BDE for HYD = 95.4 and decalin = 97.0) dissociates faster than others to form a stable tertiary carbon radical center. In HYD, the C8-H bond dissociates faster than other C2, C3, and C7-H bonds; hence, it has a lower energy barrier. For the remaining reactions of HYD (C2, C3, and C7) and decalin (C2 and C3), the abstraction barriers are nearly identical.

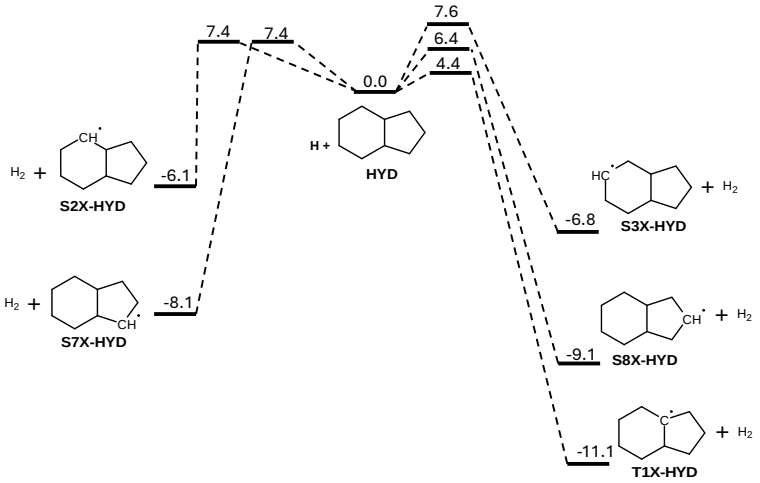


Figure 4.4: Potential energy surface for H-atom abstraction reactions of hydrindane by H atom . Energy unit: kcal/mol.

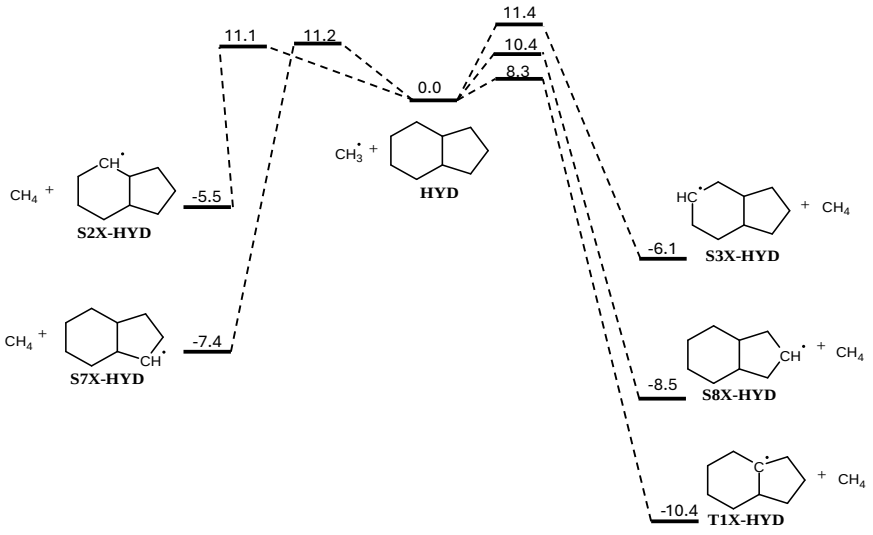


Figure 4.5: Potential energy surface for H-atom abstraction reactions of hydrindane by methyl radical. Energy unit: kcal/mol.

Table 4.4: Comparison of ring-opening isomerization via β-C-C scission of decalin radical and hydrindane radical. Energy unit: kcal/mol. Method: CBS-QB3.

Carbon radical centre	**β-C-C bond dissociation**	**HYD**	**decalin**
T1X-carbon	adjacent to tertiary carbon center	29.9	30.6
	far to tertiary carbon center	36.3	33.6
	adjacent to tertiary carbon center	33.6	-
	far to tertiary carbon center	31.6	-
S2X-carbon	adjacent to tertiary carbon center	25.9, 31.3	28.9, 35.3
	far to tertiary carbon center	28.3	29.6
S3X-carbon	adjacent to tertiary carbon center	31.6	30.0
	far to tertiary carbon center	28.3	30.5
S7X-carbon	adjacent to tertiary carbon center	33.3, 35.4	-
	far to tertiary carbon center	33.5	-
S8X-carbon	adjacent to tertiary carbon center	33.9	-

4.4.3 Decomposition and isomerization of HYD radicals

The hydrogen abstraction of the HYD results in five different HYD radicals, as illustrated in the previous section. Figures 4.6, 4.7, 4.8, 4.9 and 4.10 show the possible unimolecular dissociation and isomerization reactions (Method: CBS-QB3//B3LYP/6-311G(2d,d,p)) of all five HYD radicals that proceed either by β-C-H scission (H-elimination) or by the ring-opening isomerization via β-C-C scission, leading to the opening of the five- or six-membered ring giving alkyl radicals. Their energy barrier depends upon the C-H and C-C BDEs, and so the H elimination barriers are usually higher than the isomerization reactions. Further, during beta scission of the radical chain, the free radical cleaves two carbon atoms apart (beta-position) from the carbon radical center, resulting in the formation of an olefin (ethylene) and a primary radical with two fewer carbon atoms, and so on. The radical decomposition steps determine the product distribution during the later stages of the pyrolysis reaction. This step often competes with the isomerization step, which can lead to the formation of other cycloalkanes.

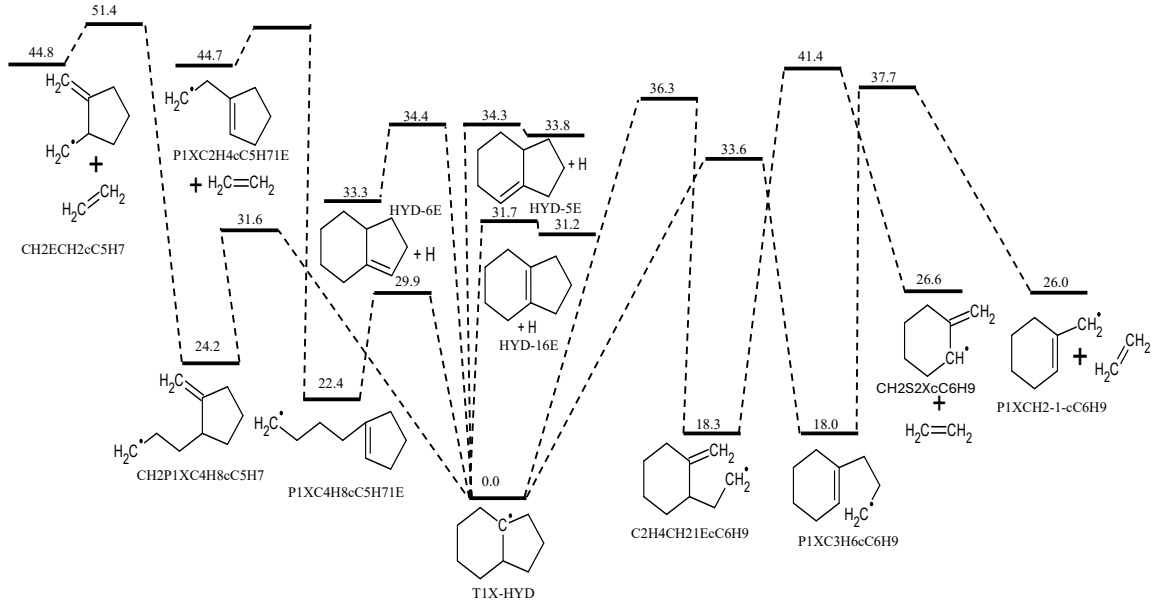


Figure 4.6: Isomerization and decomposition reactions of T1X hydrindane. Energy unit: kcal/mol.

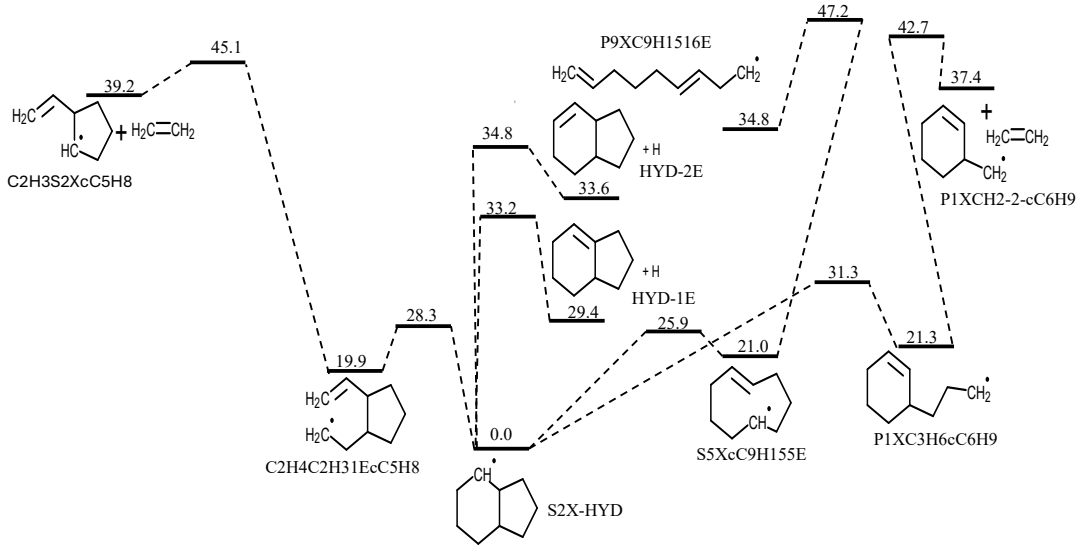


Figure 4.7: Isomerization and decomposition reactions of S2X hydrindane. Energy unit: kcal/mol.

Tables 4.4 and 4.5 show the comparison of ring-opening isomerization via β-C-C and β-C-H scission of decalin radical and hydrindane radical. In the ring-opening isomerization step, the C-C bond distance nearest to the tertiary carbon center has a lower energy barrier compared to the alternative

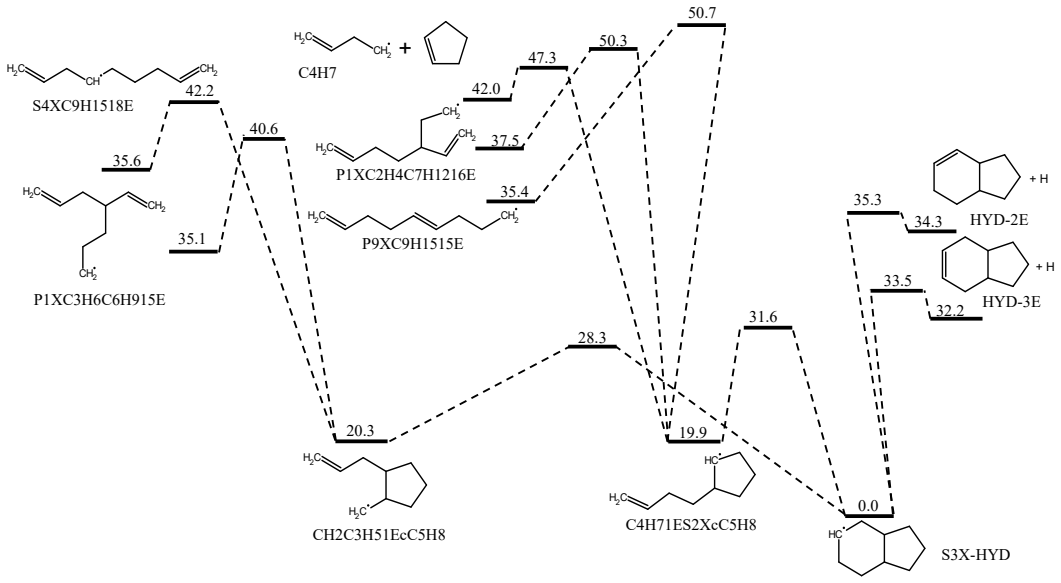


Figure 4.8: Isomerization and decomposition reactions of S3X hydrindane. Energy unit: kcal/mol.

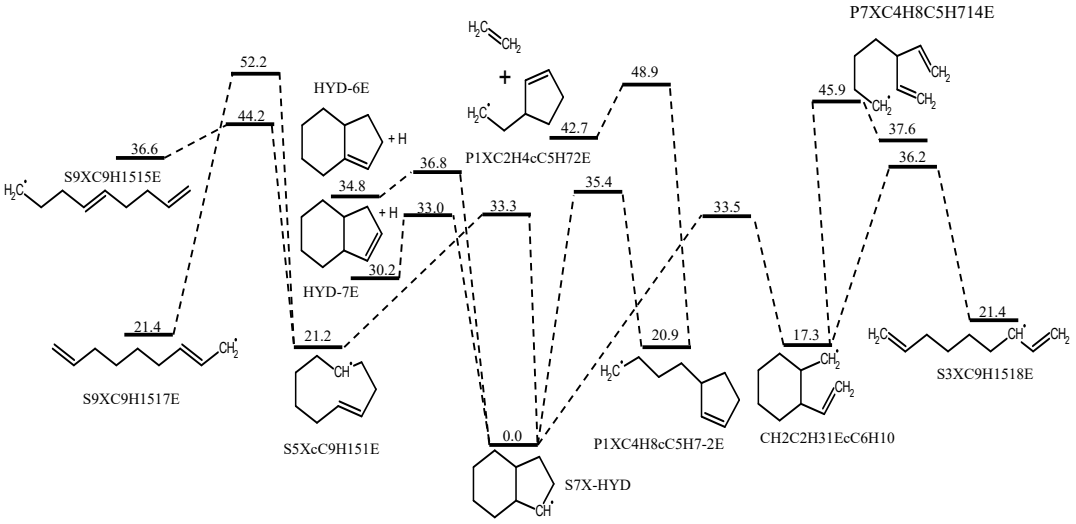


Figure 4.9: Isomerization and decomposition reactions of S7X hydrindane. Energy unit: kcal/mol.

C-C bonds in the HYD radical.

In HYD, the C-C BDE depends on which ring is opening (the C-C BDE from 5 rings is less than that from 6 rings), as mentioned in the first step. C-H elimination is not always more than the C-C bond here. The energy barrier for

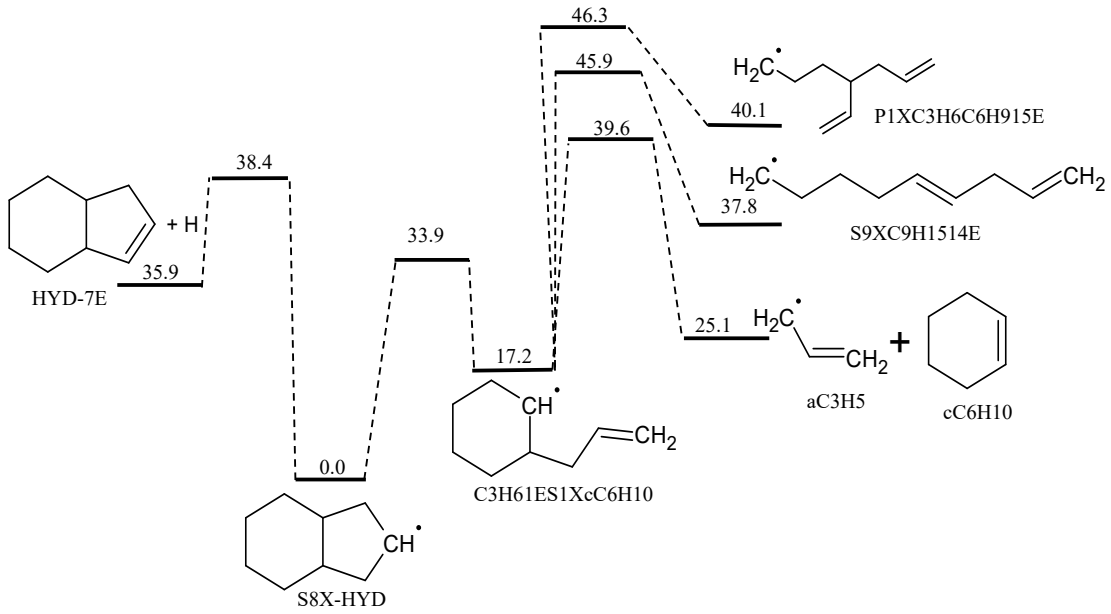


Figure 4.10: Isomerization and decomposition reactions of S8X hydrindane. Energy unit: kcal/mol.

dissociation through the β-C-H scission was higher in almost all cases.

The β-C-C scission of the HYD and decalin radical, giving cyclononenyl (25.9 kcal/mol) and cyclodecenyl (28.9 kcal/mol) radicals, have the lowest energy barrier among all the reactions. This β-C-C scission is an example of the fused C-C bond dissociation in both HYD and decalin. β-C-H bond dissociation, which leads to the formation of a double C-C bond between the fused C1-C6 position, has the lowest energy barrier in both HYD and decalin.

4.4.4 Decomposition and isomerization of hydrinene radicals

The decomposition of HYD radicals yields various hydrindene radicals, as demonstrated in the preceding section. Figures 4.11, 4.12, 4.13, 4.14 and 4.15 illustrate the potential dissociation and isomerization reactions that occur by abstraction mechanisms (Method: CBS-QB3//B3LYP/6-311G(2d,d,p)), followed by ring-opening isomerization via β-C-C scission, resulting in the cleav-

Table 4.5: Comparison of decomposition via β-C-H scission of decalin radical and hydrindane radical. Energy unit: kcal/mol. Method: CBS-QB3.

Carbon radical centre	**β-C-H bond dissociation**	**HYD**	**decalin**
T1X-carbon	adjacent to tertiary carbon center	34.3	34.7
	far to tertiary carbon center (C6-H)	31.7	32.2
	adjacent to tertiary carbon center (C9-H)	34.4	-
S2X-carbon	adjacent to tertiary carbon center T1X	33.2	34.3
	far to tertiary carbon center S8X	34.8	35.5
S3X-carbon	adjacent to tertiary carbon center S2XC-H	35.3	35.7
	far to tertiary carbon center S4XC-H	33.5	35.3
S7X-carbon	adjacent to tertiary carbon center T1X-C-H	36.8	-
	far to tertiary carbon center S3X-C-H	33.0	-
S8X-carbon	S7X-C-H	38.4	-

Table 4.6: Comparison of the lowest energy pathways between HYD and decalin radicals. Energy unit: kcal/mol. Method: CBS-QB3.

Bond dissociation	**HYD**	**decalin**
β-C-C bond dissociation	25.9	28.9
β-C-H bond dissociation	31.7	32.2

age of five- or six-membered rings to yield alkenyl radicals. Further, during beta scission of the radical chain, the free radical cleaves two carbon atoms apart (beta position) from the carbon radical center, resulting in the formation of an olefin (ethylene) and a primary radical with two fewer carbon atoms, and so on. The decomposition processes of alkenyl cyclohexane and cyclopentane radicals are obtained from the submechanisms of cyclopentane and cyclohexane, analogous to the decomposition reactions of hydrindane radicals discussed in the previous section.

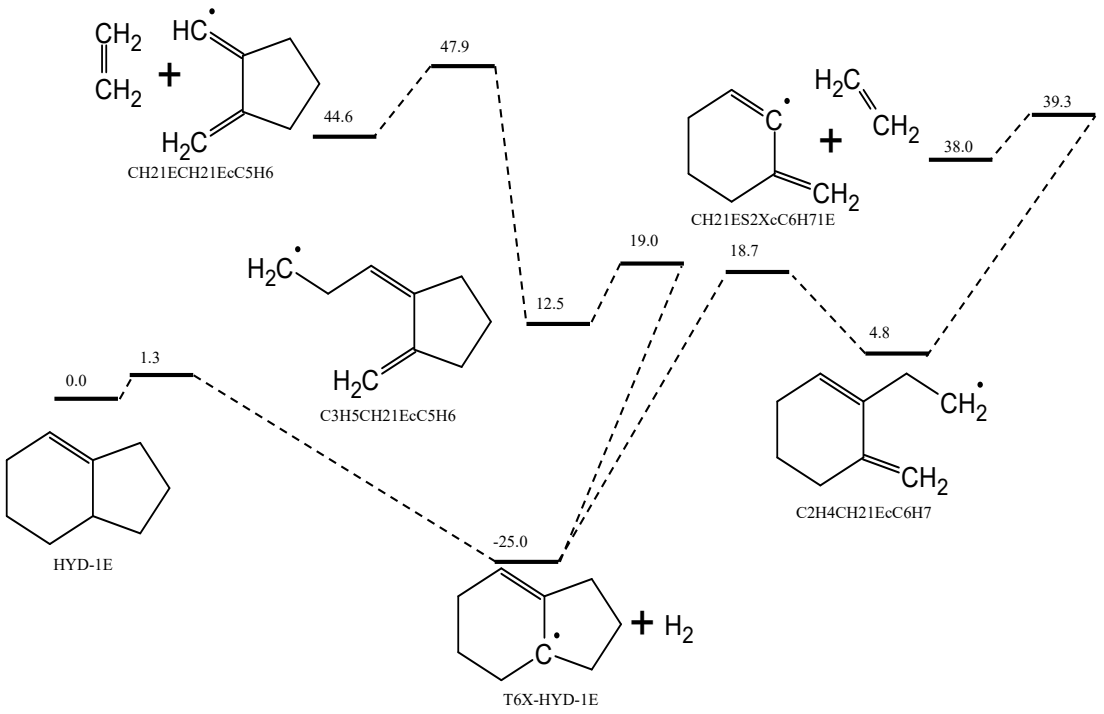


Figure 4.11: Isomerization and decomposition reactions of HYD-1E hydrindene. Energy unit: kcal/mol.

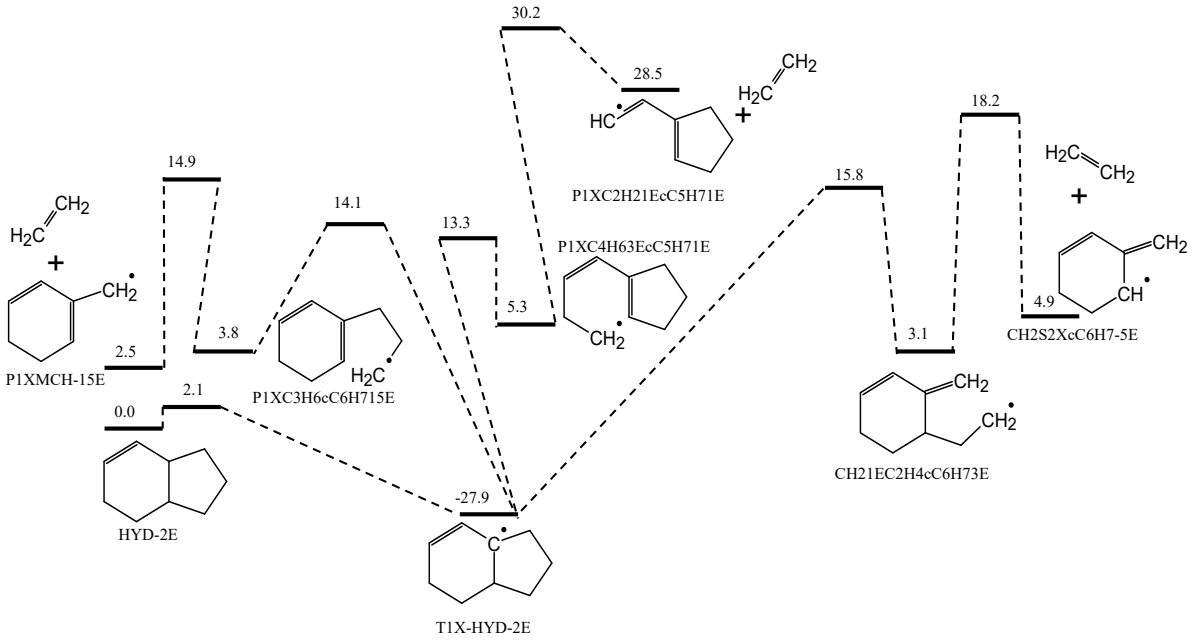


Figure 4.12: Isomerization and decomposition reactions of HYD-2E hydrindene. Energy unit: kcal/mol.

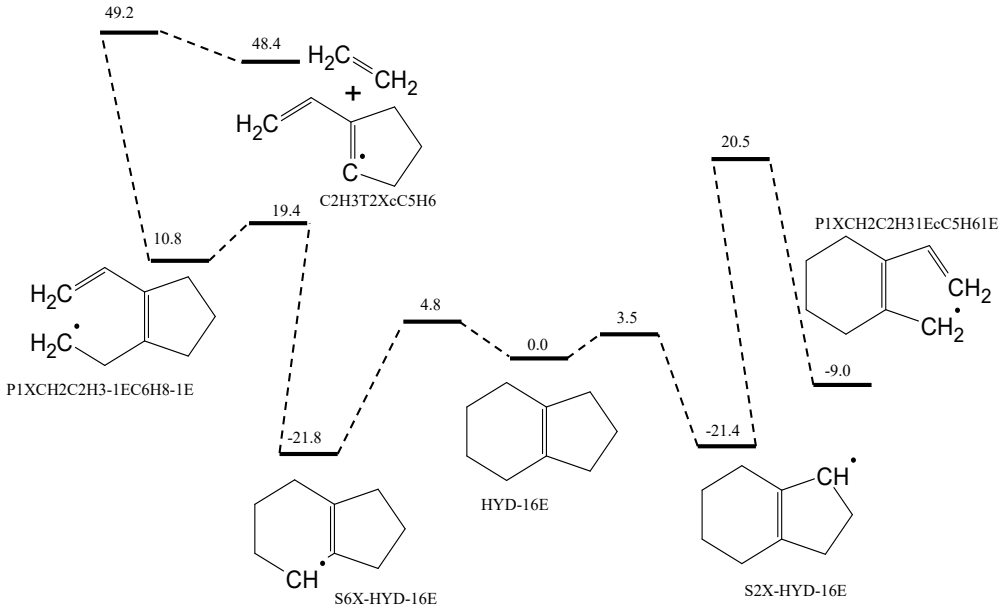


Figure 4.13: Isomerization and decomposition reactions of HYD-16E hydrindene. Energy unit: kcal/mol.

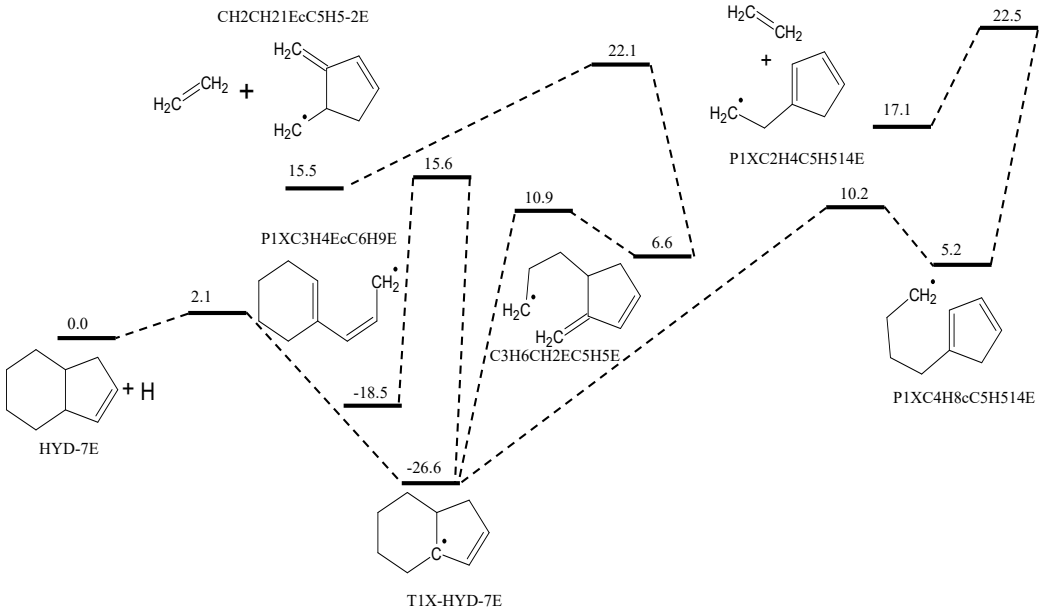


Figure 4.14: Isomerization and decomposition reactions of HYD-7E hydrindene. Energy unit: kcal/mol.

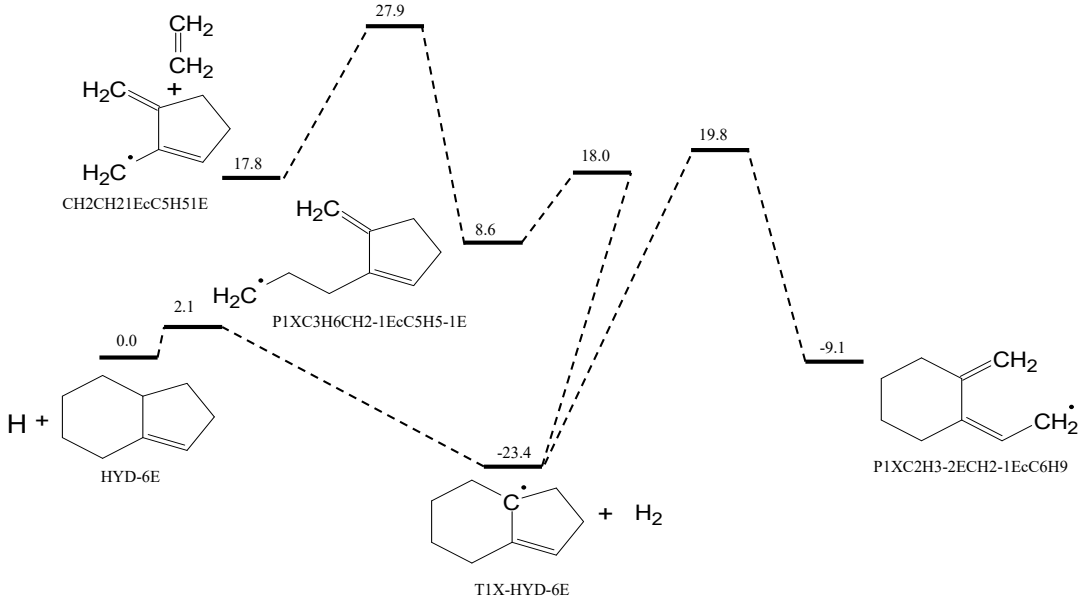


Figure 4.15: Isomerization and decomposition reactions of HYD-6E hydrindene. Energy unit: kcal/mol.

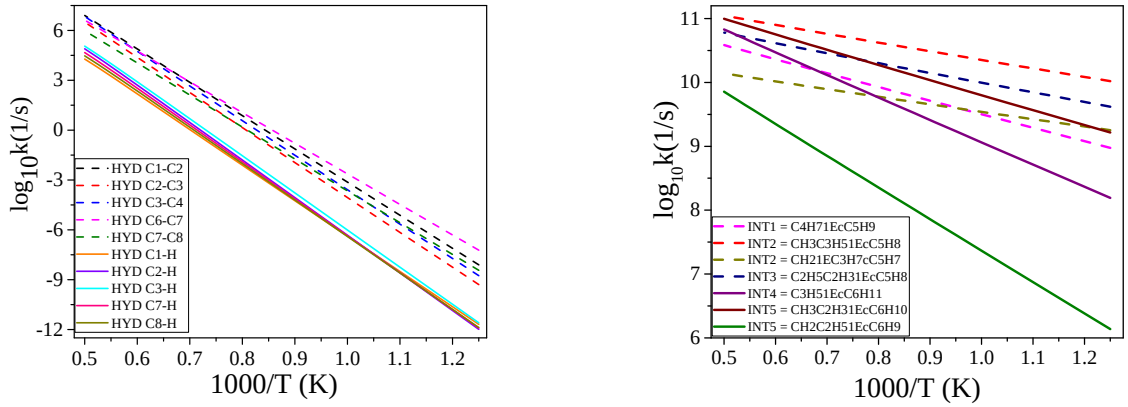
4.4.5 Rate constant calculations

The high-pressure limit (HPL) temperature-dependent rate constants were determined using conventional transition state theory (TST) for reactions with a saddle point and variational transition state theory (VTST) for barrierless reactions (no saddle point) within the temperature range of 800–2000 K. Table 4.7 shows the rate constants of the primary decomposition channels of hydrindane: unimolecular decomposition, ring-opening isomerization, and abstraction reactions of HYD.

Unimolecular decomposition and ring-opening isomerization of HYD

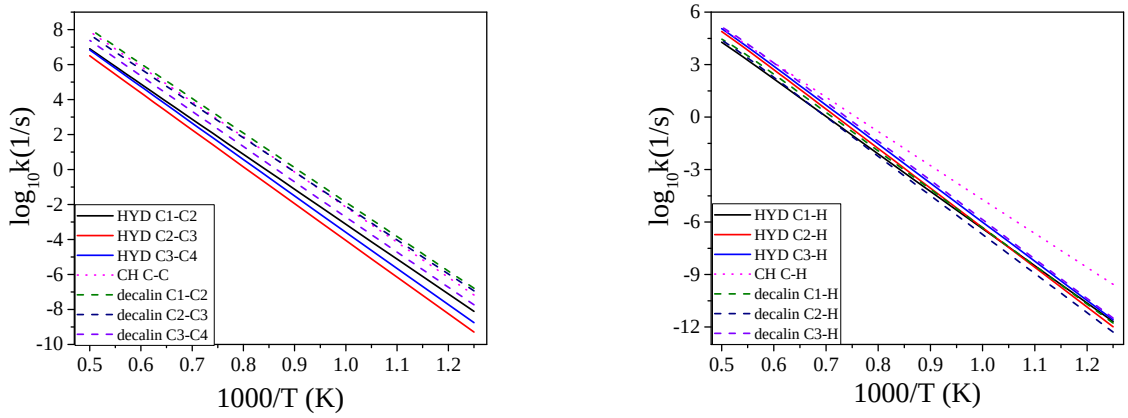
The first reaction channel is the unimolecular decomposition step (C-H bond dissociation). The reaction is an example of a barrierless reaction with no saddle point, and the stepwise relaxed bond scan was done to get the PES,

and rate constants are calculated with VTST. Figure 4.2 illustrates that the barrier height of the VTST varies from 89.8 to 98.5 kcal/mol as the C-H bond stretches from 2.5 to 3.3 A within the analyzed temperature range. Figure 4.16 compares the HPL rate constant of the unimolecular decomposition and ring-opening step of the isomerization of HYD (the first step to form biradical intermediates). A biradical intermediate is formed via the homolytic cleavage of a C-C bond, resulting in two unpaired electrons positioned on two separate carbon atoms within a single molecule. These species are highly reactive and unstable in nature, forming alkenes via intramolecular H migration in the second step with a very low energy barrier. Comparing the HPL rate constants of the unimolecular decomposition and the formation of biradical intermediates is necessary. From the figure, we can see that the ring-opening isomerization process is faster than unimolecular decomposition channels (BDE of C-C $<$ C-H). The C-C bond dissociation leading to INT4 and INT1 via C6-C7 (5-membered ring opening) and C1-C2 (6-membered ring opening), which are adjacent to the tertiary carbon atom, are the fastest processes among them.



(a) (b)

Figure 4.16: Comparison of the HPL rate constant of the unimolecular decomposition and ring-opening isomerization of HYD: the first step to form biradicals (solid lines are for C-C and dotted lines are for C-H bond dissociation) and the 2nd step of intramolecular H-migration from biradical to form alkenes (solid lines are for a 5-membered cyclic transition, and the dotted line is for a 6-membered cyclic transition.) (*a*) Rates for C-H and C-C bond dissociation. (*b*) Rates for H-migration: biradical to alkene.



(a) (b)

Figure 4.17: Comparison of the HPL rate constant of the unimolecular decomposition and ring-opening step of isomerization of HYD, decalin, and cyclohexane (first step to form biradicals). (*a*) Rates for C-H bond dissociation. (*b*) Rates for C-H bond dissociation.

Figure 4.17 shows the comparison of the HPL rate constant of the unimolecular decomposition and ring-opening step of isomerization of HYD and decalin (the first step to form biradicals). The dissociation of the decalin and CH C-C bond occurs more rapidly than that of HYD, although the rates of C-H dissociation are comparable.

H-migration

Figure 4.16 shows the HPL rate constants of the ring-opening isomerization (2nd step) of HYD (intramolecular H-migration from biradical to form alkenes). The rates for the intramolecular H-migration step are significantly higher than those for the first step, primarily due to lower energy barriers (biradical intermediates are highly reactive). In general, the 6-membered cyclic transition has higher rates as compared to the 5-membered cyclic transition. INT2=1CH3-2C3H52E-C5H8, INT3=C3H5-1ECH3C5H8 (6-membered cyclic transition), and INT5=1C2H31E-2CH3C6H10 (5-membered cyclic transition) have low energy barriers and have faster rates (H-migration from carbon chain to carbon chain). INT1=C4H7-1EC5H9 (H-transfer from carbon chain to CP

Table 4.7: High-pressure limit (HPL) rate constants of the primary decomposition channels of hydrindane: unimolecular decomposition, ring-opening isomerization, and abstraction reactions of HYD

Reaction	A (s^{-1})	Ea (cal/mol)
Unimolecular decomposition		
(R1) HYD = T1X-HYD+H	9.54E+14	97682.9
(R2) HYD = S2X-HYD+H	1.70E+16	103196.8
(R3) HYD = S3X-HYD+H	1.78E+16	101835.7
(R4) HYD = S7X-HYD+H	6.35E+15	101356.9
(R5) HYD = S8X-HYD+H	2.85E+15	99977.9
(R6) HYD = INT1	8.00E+16	91631.8
(R7) INT1 = C4H71EcC5H9	4.49E+11	9834.9
(R8) HYD = INT2	1.06E+17	96430.9
(R9) INT2 = CH3C3H51EcC5H8	5.30E+11	6272.8
(R10) INT2 = CH21EC3H7cC5H7	5.37E+10	5436.0
(R11) HYD = INT3	1.70E+17	95222.6
(R12) INT3 = C2H5C2H31EcC5H8	3.50E+11	7079.2
(R13) HYD = INT4	6.96E+15	84517.6
(R14) INT4 = C3H51EcC6H11	3.83E+12	16104.3
(R15) HYD = INT5	3.84E+15	88007.1
(R16) INT5 = CH3C2H31EcC6H10	1.51E+12	10874.6
(R17) INT5 = CH2C2H51EcC6H9	2.12E+12	22693.8
Abstraction reactions		
(R18) HYD+H = T1X-HYD+H2	2.44E+14	8033.9
(R19) HYD+H = S2X-HYD+H2	6.44E+14	11115.6
(R20) HYD+H = S3X-HYD+H2	6.44E+14	11326.1
(R21) HYD+H = S7X-HYD+H2	4.07E+14	11027.0
(R22) HYD+H = S8X-HYD+H2	1.80E+14	10002.8
(R23) HYD+CH3 = T1X-HYD+CH4	7.05E+12	14879.8
(R24) HYD+CH3 = S2X-HYD+CH4	5.85E+13	17732.8
(R25) HYD+CH3 = S3X-HYD+CH4	7.07E+13	18037.2
(R26) HYD+CH3 = S7X-HYD+CH4	2.52E+13	17779.7
(R27) HYD+CH3 = S8X-HYD+CH4	1.30E+13	16879.7

ring) has a lower rate due to a higher energy barrier than other 6-membered cyclic TS. INT2=1CH21E-2C3H75C5H7 has the lowest A factor (5.37E+10), which is why it exhibits a lower rate despite having a very low energy barrier. (H-transfer from ring to carbon chain). INT5=1C2H5-2CH2EC6H9 (H-transfer from the CH ring to the carbon chain) has the lowest rate due to a very high energy barrier.

H-abstraction reaction by H and CH_3 radical

Figure 4.18 illustrates the high-pressure Arrhenius plot for the rate constants of the H-abstraction reaction via H and CH_3 radicals for hydrindane (Upon the formation of an open-chain structure, normal β-scission produces methyl radicals). Figure 4.19 shows the comparison of the rate constant of H-abstraction reactions of HYD and decalin by H and CH_3 radicals. The rate constant for H-abstraction from decalin and hydrindane by a hydrogen atom exceeds that of H-abstraction by a methyl radical. The H abstraction at the tertiary carbon has the lowest energy barrier. As expected, the rate constant for H abstraction reactions by the H radical at the tertiary carbon in hydrindane is the highest. Whereas in methyl abstraction, it is not the case (low A factor). In the case of decalin, the A factor is lower for both the H atom and methyl abstraction. The rate constant for the H-atom and CH_3 abstraction at the tertiary carbon in hydrindane is lower than that of decalin in both cases. The rate constants for S2X and S3X carbon are almost identical for both HYD and decalin due to similar activation energies and A factors. The lowest rate for the HYD is the H abstraction from S8X carbon.

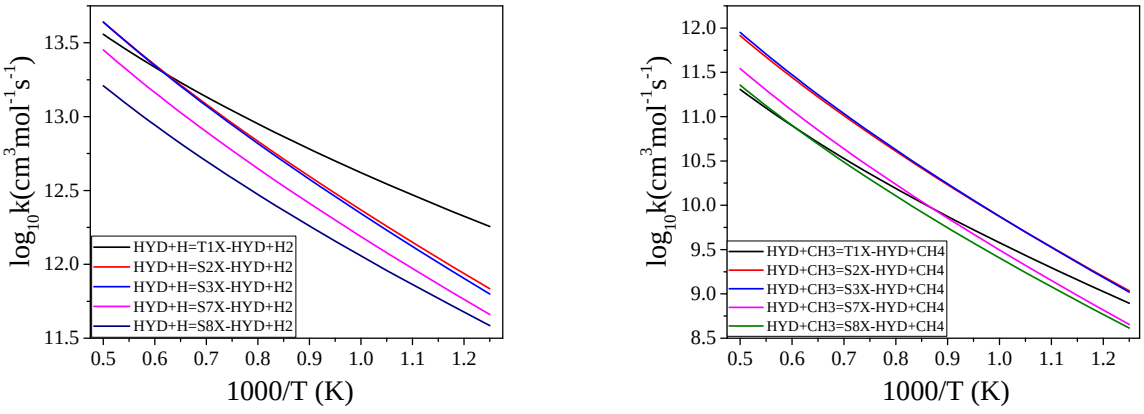


Figure 4.18: HPL rate constant of H-atom abstraction of HYD from H and CH_3 radical.

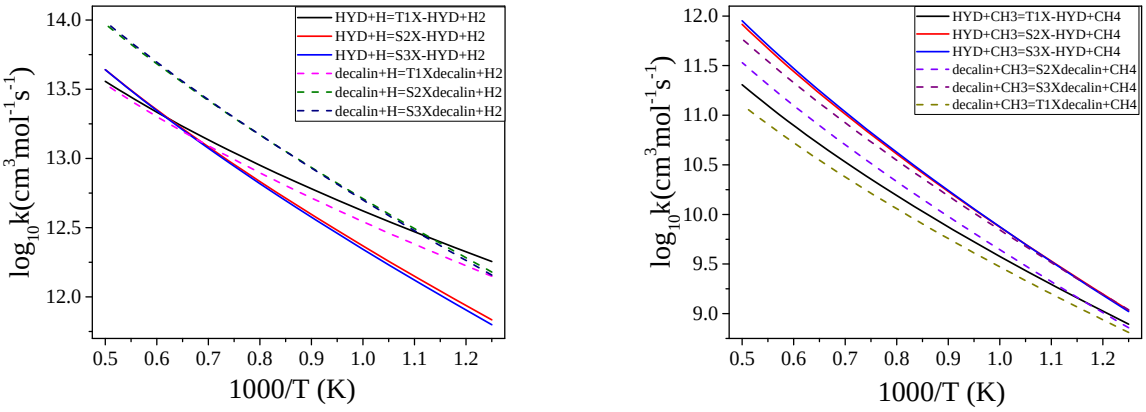


Figure 4.19: Comparison of the rate constant of H-abstraction reactions of HYD and decalin by H and CH_3 radicals. The solid line represents HYD, and the dotted line represents decalin.

4.5 Experiment results and model validation

In pyrolysis investigations performed at temperatures ranging from 1000 to 1550 K and corresponding pressures of 12.8 to 23.3 bar, a total of 17 species were identified. C1–C5 species that are detected are methane (CH_4), acetylene (C_2H_2), ethylene (C_2H_4), ethane (C_2H_6), allene (aC_3H_4), propene (C_3H_6), propyne (pC_3H_4) 1,3-butadiene (C_4H_6), 1-butene (C_4H_8), cyclopentene (cC_5H_8), cyclopentadiene (C_5H_6), methylcyclopentadiene ($C_5H_5CH_3$). Benzene (A1), toluene (A1CH3), and styrene (A1C2H5) are the aromatic compounds detected during the experiment.

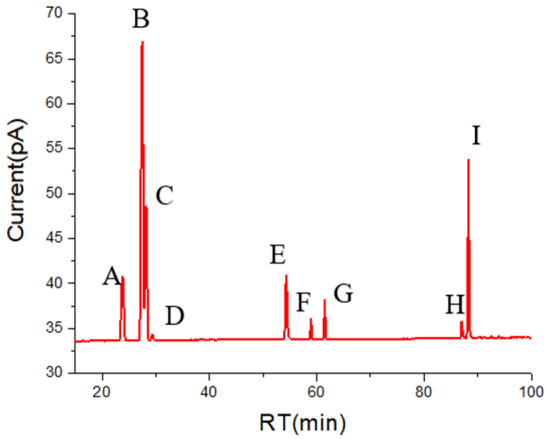


Figure 4.20: Chromatogram from GC front-FID (lower boiler species) (HP-PLOTQ-column). A= Methane, B= Ethylene, C= Acetylene, D= Ethane, E= Propylene, F=Allene, G=Propyne, H=Butene, I=1,3-Butadiene.

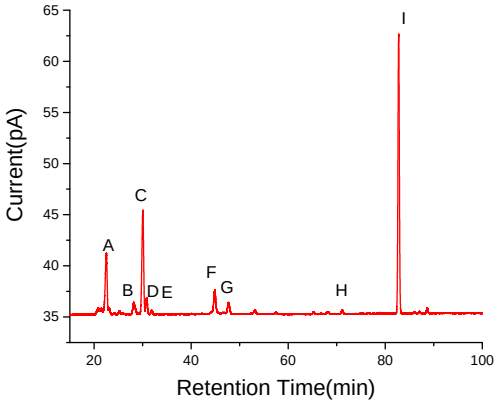


Figure 4.21: Chromatogram from GC back-FID (higher boiler species) (HP-5 column). Peaks are assigned to A = Cyclopentadiene, B = Methylcyclopentadiene, C = Benzene, D = Cyclohexadiene, E = Cyclohexene, F = Toluene, G = Methylcylohexadiene, H = Styrene, and I = HYD.

The carbon balance method estimates the initial reactant concentration under the assumption that all carbon is retained in the gas phase, as demonstrated in the prior study. [257]. Using the carbon balance method,

$$[HYD]_0 = [HYD]_t + \sum_{i=1}^{17} \frac{n_i[P_i]_t}{9}$$

In Equation 1, $[HYD]_0$ denotes the initial concentration of trans-hydrindane, $[HYD]_t$ indicates the concentration of hydrindane at time t, n_i represents the

number of carbon atoms in the ith product, and $[P_i]_t$ signifies the concentration of the ith product at time t.

The distributions of the normalized concentrations of reactants and all products, including both minor and major species, within the experimental temperature range, as determined by kinetic modeling, are presented and analyzed in the following sections. To gain insight into the chemistry governing the decomposition of HYD and the formation of aromatic chemicals, rate of production (ROP) analysis and sensitivity analysis were conducted at different temperature and pressure conditions.

4.5.1 Primary decomposition of hydrindane

Figure 4.22 depicts the experimental and simulated mole fraction distributions of HYD. The current model accurately forecasts general trends in HYD decomposition in relation to temperature. HYD begins to degrade at approximately 1150 K and is entirely consumed at temperatures beyond 1500 K. Figure 4.23 illustrates the principal mechanisms of HYD decomposition, including unimolecular dissociation (C-H and C-C bond dissociation) and hydrogen abstraction processes predominantly involving H and CH_3 radicals. During the initial consumption processes of HYD, five distinct hydrindane radicals are generated: S2X-HYD, S3X-HYD, S7X-HYD, and S8X-HYD (secondary radicals), and T1X-HYD (tertiary radical).

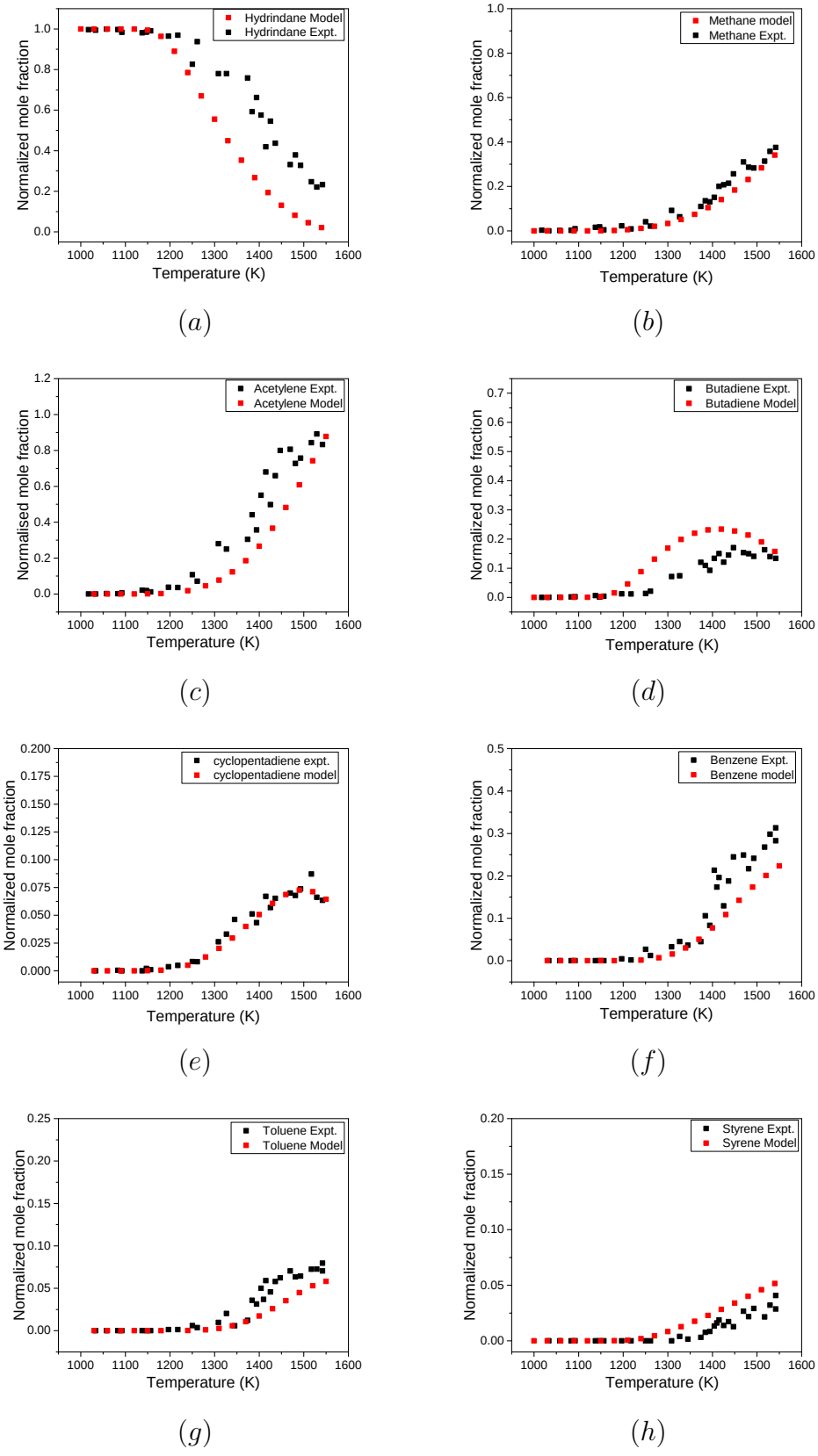


Figure 4.22: Experimental (symbols) and modeling (lines) results of some major species of HYD pyrolysis. Normalization mole fraction for reactant $= [HYD]_t/k[HYD]_0$; Normalization mole fraction for products $=[P_i]_t/k[HYD]_0$; where $k = [HYD]_t/[HYD]_0 + \sum_{i=1}^{17} \frac{[P_i]_t}{[HYD]_0}$

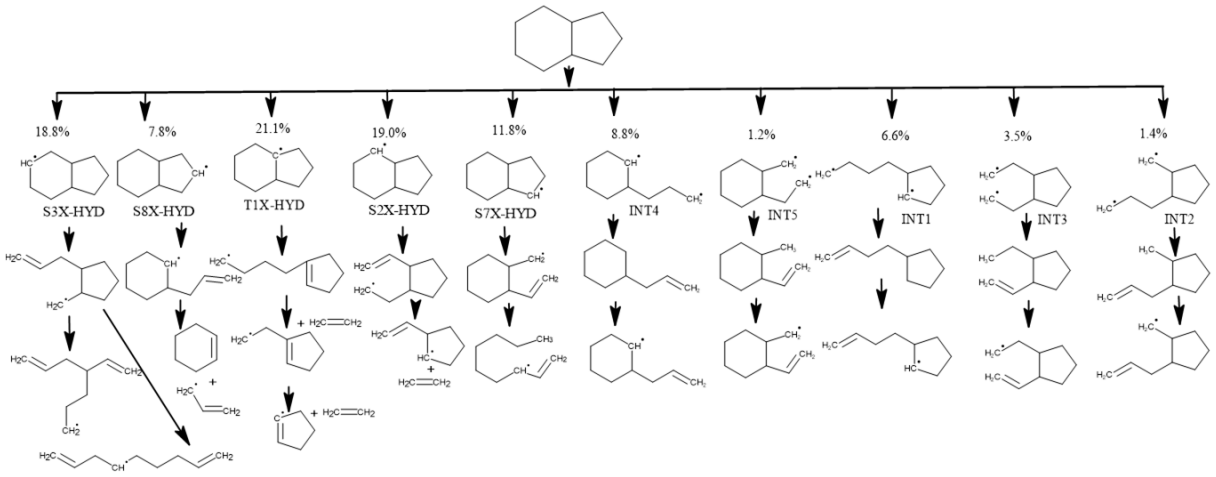


Figure 4.23: Reaction pathways using HYD at a temperature of 1400 K, achieving 80% conversion of HYD. The figure with the arrow indicates the respective percentage contribution to the overall contributions. The initial steps for hydrindane radicals are also shown.

Figure 4.23 shows the reaction flux of primary intermediates (radicals) generated from the initial decomposition of HYD that has been performed at 1400 K to better understand the complex mechanisms of HYD pyrolysis. The reaction flux analysis of HYD at 1400 K, as predicted by the present model, is illustrated in the figure, corresponding to a conversion of around 80%. The figure illustrates that HYD undergoes decomposition and isomerization, predominantly producing hydrindane radicals, with T1X-HYD, S2X-HYD, and S3X-HYD as the primary products resulting from abstraction. The hydrogen atom abstraction reactions substantially consume the reactant throughout all temperature and pressure ranges. The C–C bond dissociation reactions are more favorable than C–H bond dissociation reactions among dissociation processes, due to the significantly lower bond dissociation energies (BDEs) of C–C bonds relative to C–H bonds in cycloalkanes during decomposition (refer to 4.1). The biradical intermediates formed from the HYD constitute almost 21.5% of the HYD consumption, as the figure shows.

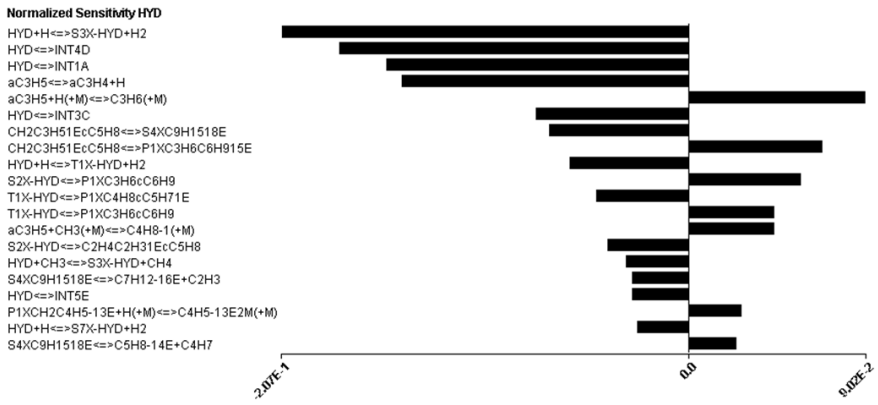


Figure 4.24: Normalized sensitivity analysis of HYD during HYD pyrolysis at 1400 K, with an HYD conversion rate of approximately 80%.

A sensitivity study of HYD has been performed to better understand the influence of unimolecular decomposition and H-atom abstraction processes on HYD consumption. The sensitivity study indicates that the most sensitive reaction is the C-C dissociation of HYD, followed by H-abstraction reactions that produce S3XHYD. HYD is predominantly utilized in unimolecular dissociation reactions and H-abstraction reactions involving hydrogen atoms and methyl radicals, as well as other radicals, in pyrolysis reactions. The beneficial impact of these reactions on HYD consumption came from their role as the primary consumption routes for HYD. Consequently, hydrogen atom abstraction mechanisms of HYD transpire rapidly with the incorporation of more hydrogen atoms or methyl radicals into the system. The decomposition of five C_9H_{15} HYD radicals primarily occurs through β–C–C cleavage mechanisms, resulting in the ring opening of the five- or six-membered rings of the radicals. The alkenyl cyclopentane/cyclohexane radicals are not discovered during post-shock gas chromatography examination due to their limited lifetimes and high reactivity. The breakdown of these monocyclic radicals will ultimately provide aromatic compounds as well as smaller alkenes and alkanes, which will be addressed in the subsequent two sections.

4.5.2 Formation of C1–C5 species

This study examined various C1–C5 species, including alkanes, alkenes, and alkynes, specifically methane, ethene, and acetylene. The product concentration profiles indicate that methane (CH_4), acetylene (C_2H_2), and ethylene (C_2H_4) are the predominant products resulting from the decomposition of HYD. Following ethylene, concentrations of methane and acetylene are also shown to be high. C3 compounds, including allene (aC_3H_4), propene (C_3H_6), and propyne (pC_3H_4), exhibit similar trends.

1,3-butadiene (C_4H_6), vinylacetylene (C_4H_4), and but-1-ene (C_4H_8) are C4 compounds produced during the decomposition of HYD, but in lesser quantities. Cyclopentene (C_5H_8) and cyclopentadiene (C_5H_6) are important cyclic C5 compounds that begin formation at the same temperature as aromatic benzene formation (1250 K), peaking about 1400 K before subsequently decreasing with temperature.

In summary, the ring-opening isomerization step of cyclohexyl/cyclopentyl radicals generates a diverse range of alkenyl radicals.

4.5.3 Formation of benzene, toluene, and styrene

Benzene, styrene, and toluene are the aromatic products found in the HYD pyrolysis. Aromatics like benzene and toluene are predominantly generated through the addition of resonance-stabilized radicals. Resonance-stabilized radicals like allyl, propargyl, butadienyl, phenyl radical, and benzyl radical are thought to be crucial in the pyrolysis conditions that lead to the synthesis of aromatics. These radicals have longer lives than ordinary radicals, which allows them to build up to comparatively high concentrations. Recombination

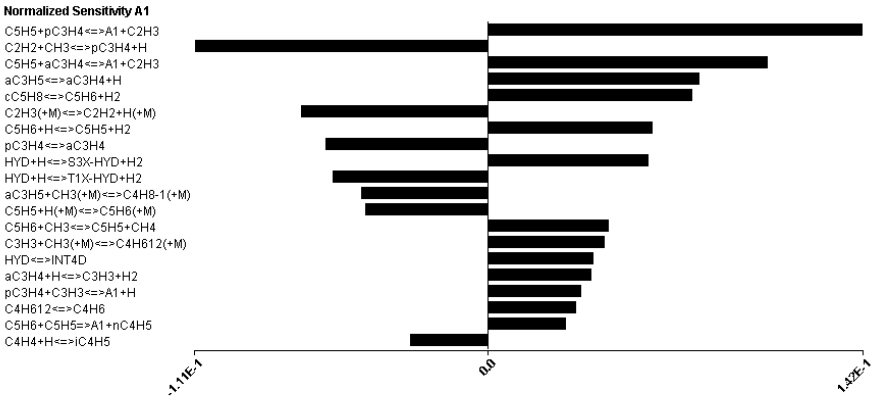


Figure 4.26: Normalized sensitivity analysis of benzene during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85 %.

reactions with other radicals or intermediates result in an increase in molecular weight and are significant consumption pathways for these resonance-stabilized radicals.

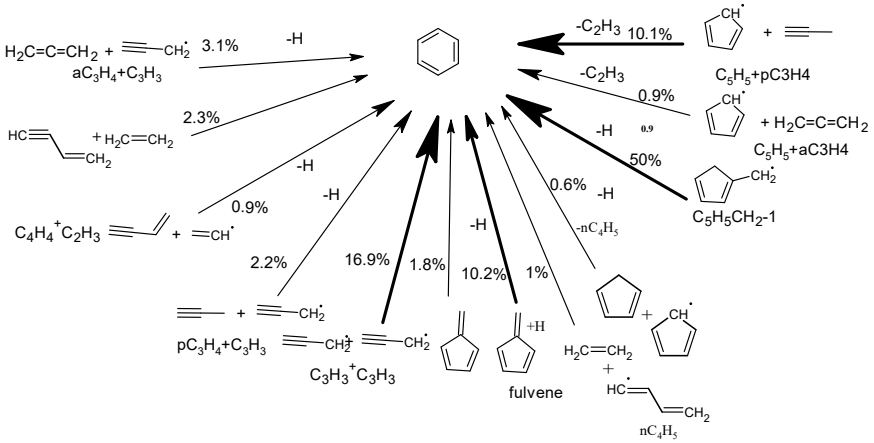


Figure 4.25: Investigation of chemical pathways for benzene synthesis during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85 %.

For HYD, the major contribution, almost 60% comes from the cyclopentadiene and methylcyclopentadiene radical reactions. Benzene is also produced via the self-recombination process of propargyl radicals (C_3H_3+C_3H_3)(17%), the combination of propargyl radicals with allene and propyne (C_3H_3+C_3H_4-A, C_3H_3+C_3H_4-P).

Fulvene, an important intermediate in the production of benzene, signif-

icantly contributes to benzene formation, accounting for 13% of the total production. It is formed by various processes, such as the addition of propargyl radicals (C_3H_3+ C_3H_3), as well as through reactions between propargyl and allyl radicals (C_3H_3+C_3H_5-A) and between acetylene and 1,3-butadiene radicals (C_4H_5-N + C_2H_2) and (C_4H_5-I + C_2H_2). The sensitivity analysis reveals that cyclopentadiene, allene, and propene radicals are the most significant radicals involved in the synthesis of benzene.

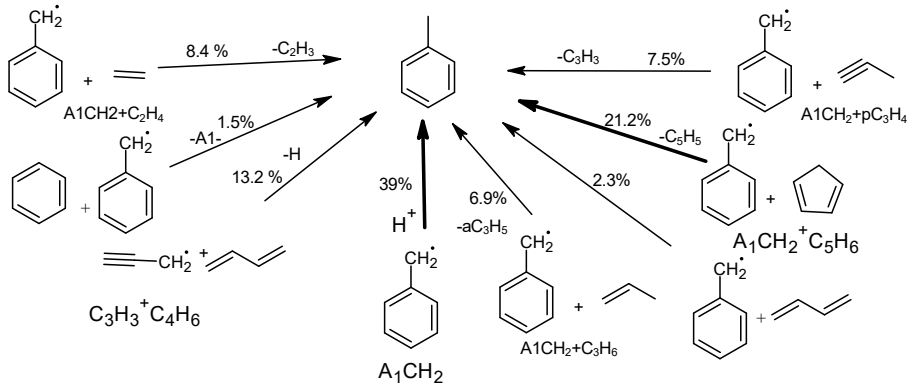


Figure 4.27: Investigation of chemical pathways for toluene synthesis during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85%.

The dominant source of toluene is the association of an H-atom with the benzyl radical (A1CH2) from the various H-atom sources (H-atom (39%), C3H6 (6.9%), pC3H4 (7.5%), and C2H4). Another important reaction for toluene formation is the addition of resonance-stabilized radicals, such as the reaction of propargyl radical with vinylacetylene (C3H3 + C4H4) (13.2%). The sensitivity analysis further reveals that benzyl and propargyl radicals are the most significant elements in toluene synthesis.

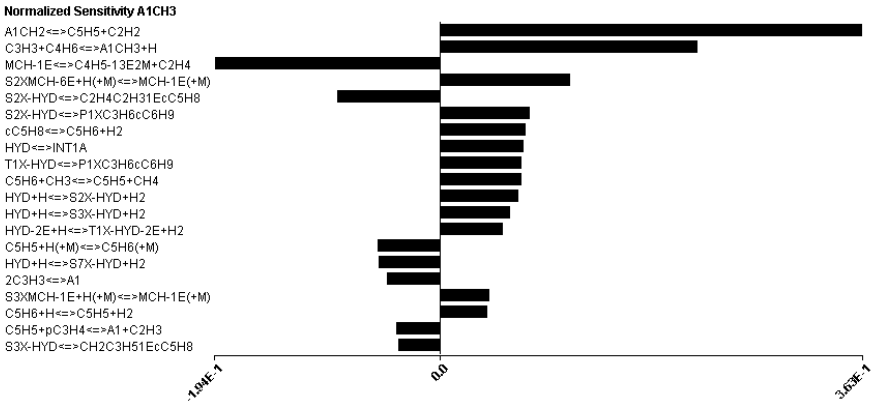


Figure 4.28: Normalized sensitivity analysis of toluene during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85%

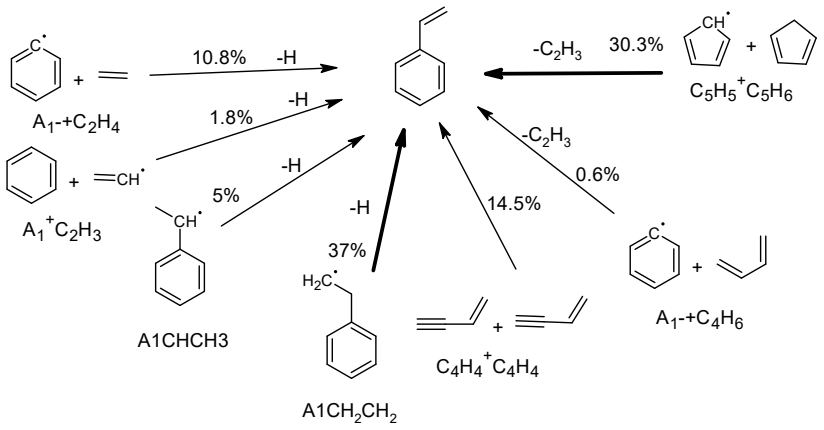


Figure 4.29: Investigation of chemical pathways for styrene synthesis during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85 %.

Styrene is produced through multiple channels. The dominant channels for styrene formation are the H elimination from the A1CH2CH2 (2-phenylethyl) radical (37%) and the addition of C5H6 (cyclopentadiene) to the C5H5 cyclopentadienyl radical (30.3%). The addition of an ethene to the phenyl radical is another important route (10.8 %), and so is the addition of two C4H4 (vinylacetylene) molecules (14.5%).

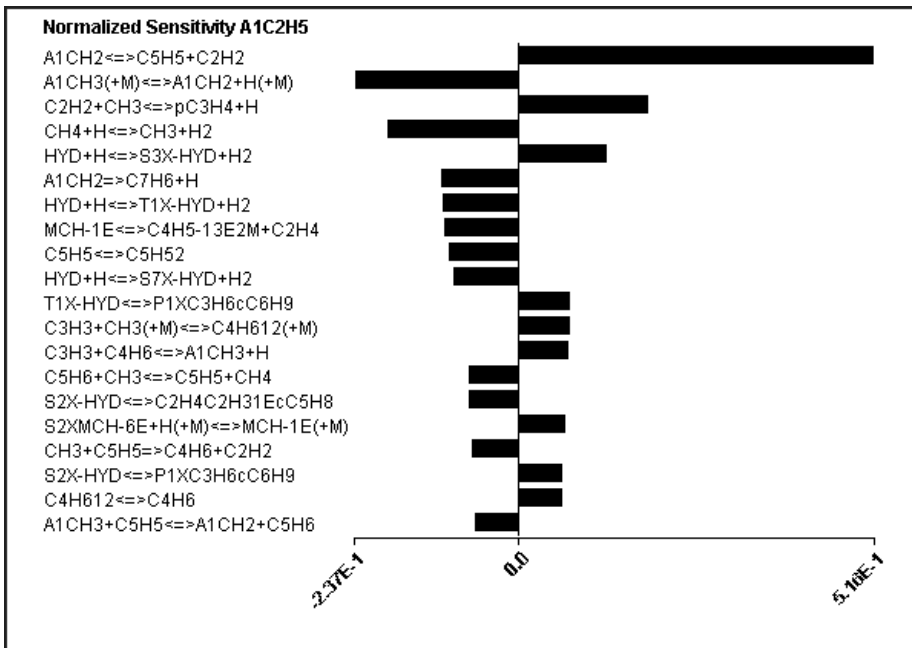


Figure 4.30: Normalized sensitivity analysis of styrene during HYD pyrolysis at 1425 K, with an HYD conversion rate of approximately 85%

4.5.4 Rate constant of the overall decomposition of HYD

The overall rate coefficient for the thermal decomposition of HYD has been determined throughout the temperature range of 1050 K to 1550 K using the following equation.

$$k = -\frac{1}{t} ln \frac{HYD_t}{HYD_0}$$

In this context, t represents the reaction time (dwell time), HYD_0 denotes the initial concentration of HYD, and HYD_t indicates the concentration of HYD after time t. The rate constant expression is derived from the linear fitting of the data presented in Figure 4.31.

$$k(s^{-1}) = 10^{8.1 \pm 0.25} exp \frac{(-34.6 \pm 1.5) kcal/mol}{RT}$$

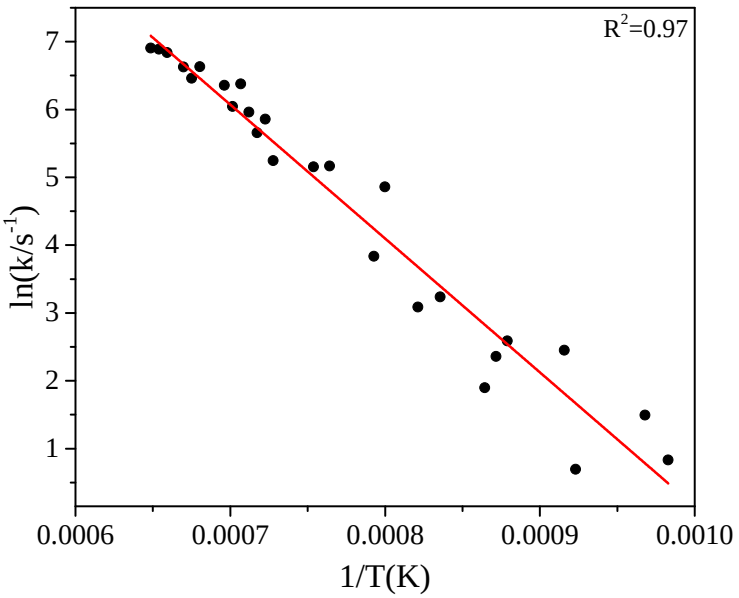


Figure 4.31: Arrhenius plot of the overall decomposition of HYD

4.6 Conclusion

This study provides an in-depth examination of the single-pulse shock tube investigation of hydrindane (C_9H_{16}), a representative bicyclic compound, under laboratory conditions that simulate environments characteristic of combustion scenarios (temperature 1000-1550 K and pressure range 12.8-23.3 bar).

The study was conducted in two parts.

1. Computation: The initial step in the thermal decomposition of HYD involves the dissociation of the C-C bond and the C-H bond. The ring-opening isomerization process (C-C bond scission) has a lower energy barrier than the unimolecular dissociation pathway (C-H bond scission). The bicyclic alkanes will dissociate more rapidly than their corresponding cycloalkanes (for instance, HYD will dissociate more easily than CP and CH, while decalin will dissociate more quickly than CH); additionally, HYD will dissociate faster than decalin. In the second stage, the

biradicals facilitate intramolecular hydrogen migration, resulting in the generation of alkenes. The energy barriers for the H migration are dependent upon six- or five-membered cyclic transition states, which are determined based on the CH or CP ring of hydrindane. A six-membered cyclic transition state is more favorable than a five-membered one due to less ring strain. The locations of carbon atoms (secondary and tertiary), the C-H BDE, and the type of H-abstraction (via H or methyl radical) substantially affect the H-abstraction reaction. H-abstraction at the tertiary carbon, leading to a tertiary carbon radical center via an H radical, has the lowest energy barrier for both HYD and decalin. The decomposition and isomerization of hydrindane radicals generate alkenyl cyclohexane and cyclopentane radicals, which, upon further decomposition, generate a variety of hydrocarbons.

Furthermore, the HPL temperature-dependent rate constants for HYD decomposition were calculated over a temperature range of 800 to 2000 K, employing the VTST and TST methods based on quantum chemistry calculations. The calculations indicate that the competition between unimolecular dissociation (C-H scission) and ring-opening isomerization pathways is strongly affected by temperature. The ring-opening channels of HYD dominate over the unimolecular decomposition step across the temperature range. The rate constant for the H-abstraction reaction by the H radical at the tertiary carbon in HYD represents the most significant abstraction reaction. The HPL rate constants for all elementary reactions indicated in the PES diagrams have been determined using the Arrhenius expression across a temperature range of 800-2000 K, which is relevant for chemical kinetic modeling of the pyrolysis of HYD. Finally, a detailed kinetic model for HYD has been developed based on the above-mentioned

calculations. The rate parameters of HYD have been further utilized to examine the experimental results from a shock tube study of HYD, as presented in the experimental part of this study.

2. This study examines the pyrolysis of HYD by analyzing species distribution in the post-shock mixture within the shock tube, across a temperature range of 1000–1550 K and pressures from 12.8 to 23.3 bar.

A range of pyrolysis products was identified and quantified, with particular importance on abundant products such as methane, ethylene, acetylene, and cyclic C6- and C7-intermediates (including benzene, 1,3-cyclohexadiene, cyclohexene, and toluene, among others). Among C1–C5 species, the predominantly produced compounds are methane, acetylene, ethylene, propene, 1,3-butadiene, 1-butene (C4H8-1), and 1,3-cyclopentadiene (C5H6). Benzene is the predominant aromatic compound, with toluene and styrene occurring in lesser quantities. The rate of production (ROP) and sensitivity analysis of HYD under pyrolysis conditions have been investigated, with an emphasis on the unimolecular dissociation/initial decomposition stages of HYD, as well as the formation of aromatics, as determined by kinetic simulations. From the reaction pathway analysis, we conclude that the decomposition of HYD originates with C–C bond dissociation; however, H-atom abstraction processes are most important for the consumption of HYD. The pyrolysis conditions that result in aromatics, such as benzene, styrene, and toluene, require the presence of resonance-stabilized radicals, including propargyl, phenyl, and benzyl radicals. Finally, the overall rate constant for the decomposition of HYD was calculated to be

$$k(s^{-1}) = 10^{8.1\pm0.25} exp \frac{(-34.6 \pm 1.5) kcal/mol}{RT}$$

The experimental data presented, along with the computational analysis and kinetic model discussed in this chapter, aim to promote further investigations into the detailed pyrolysis and oxidation study of similar bicyclic compounds. The similarity in properties with decalin and the product's similarity suggest that this could be used as a surrogate for a bicyclic compound in conjunction with decalin.

Chapter 5

Unimolecular decomposition of methyl cyclopentane

Abstract of the chapter

Alkylated cyclopentane, analogous to alkylated cyclohexane, is a typical component found in fuels, particularly in naphtha, gasoline, and jet fuels. Methylcyclopentane (MCP) (C_6H_{12}) is a representative of monoalkylated five-membered ring cycloalkanes and an isomer of cyclohexane.

The thermal decomposition of MCP at elevated temperatures in an argon bath gas was conducted using a single-pulse chemical shock tube (CST-1) facility in our laboratory. Experiments were conducted within a temperature range of 950-1600 K and a corresponding pressure range of 10-25 bar, with a dwell time of 1.40 to 1.64 ms. The post-shock products were analyzed using gas chromatography (GC) coupled with flame ionization detection (FID) and mass spectroscopy (MS).

A comprehensive kinetic model was developed based on existing chemical kinetic models, utilizing quantum chemistry techniques and rate calculations. The thermal decomposition of MCP has been examined using CASSCF/MRCI

(multireference) and CBS-QB3 (single reference) theoretical methods. Unimolecular dissociation leading to the generation of the cyclopentyl and methyl cyclopentyl radicals by the loss of a methyl radical and H radical, ring opening to hexene and methylpentene (isomerization), the abstraction of an H-atom from MCP, and the decomposition and isomerization of methyl cyclopentyl radicals. A comparison with ethylcyclopentane (ECP) is conducted, similar to that for the aforementioned reactions, to evaluate the differences among various monoalkylated cyclopentanes. The high-pressure limit (HPL) rate constants for reactions without a saddle point are determined using variational transition-state theory (VTST). On the other hand, rate constants for the remaining reactions, characterized by a single saddle-point transition state, are derived from conventional transition-state theory (TST) within a temperature range of 800–2000 K. A comprehensive MCP kinetic model was developed, integrating reaction pathways based on existing literature. The updated model was validated against the mole fraction profiles of pyrolysis species confirmed in this study.

A range of pyrolysis products was identified and quantified, with particular emphasis on abundant products such as methane, ethylene, acetylene, and aromatic products, including benzene and toluene. The rate of production (ROP) and sensitivity analysis of MCP under pyrolysis conditions have been investigated, with an emphasis on the unimolecular dissociation/initial decomposition stages of MCP, as well as the formation of benzene, as determined by kinetic simulations. From the reaction pathway analysis, we conclude that for the decomposition of MCP, C–CH_3 bond dissociation and H-atom abstraction reactions are the most important reaction pathways for the consumption of MCP. The pyrolysis conditions that result in aromatics, such as benzene and toluene, require the presence of resonance-stabilized radicals, including allyl,

propargyl, butadienyl, phenyl, and benzyl radicals. Finally, the overall rate constant for the decomposition of MCP was calculated to be

$$k(s^{-1}) = 10^{11.3\pm0.3} exp \frac{(-39.1 \pm 1.7) kcal/mol}{RT}$$

5.1 Background

Methylcyclopentane (MCP) is chosen as the surrogate component for studying transportation fuels, such as naphtha/gasoline [132]. This study aims to address the gap in the literature regarding the theoretical and experimental study of the thermal decomposition of MCP in shock tubes at high-pressure and high-temperature conditions. The previous mechanisms of high-temperature pyrolysis and oxidation reactions of MCP include the rate constants for the initial decomposition pathways of MCP, derived by comparing with the reactions of cyclopentane (CPT) or methylcyclohexane (MCH). Therefore, it is essential to conduct quantum chemistry and rate calculations for all initial reactions while developing the kinetic mechanism for this study.

The unimolecular decomposition and ring-opening isomerization channels also represent the initial reactions in the combustion process of MCP. Consequently, examining the kinetics of these channels serves as the foundation for studying MCP and the combustion of alkylated cyclopentanes, such as ECP, IPCP, and others. Additionally, the impact of side chain length, such as MCP versus ECP, IPCP (isopropyl cyclopentane), etc., on the formation of aromatic compounds can be understood. The decomposition of alkyl cycloalkanes, such as MCP and ECP, can occur in three ways: The unimolecular reaction may occur through the elimination of a C-H bond, loss of an alkyl group, i.e., the methyl or ethyl side chain, or ring-opening isomerization to hexene or heptene

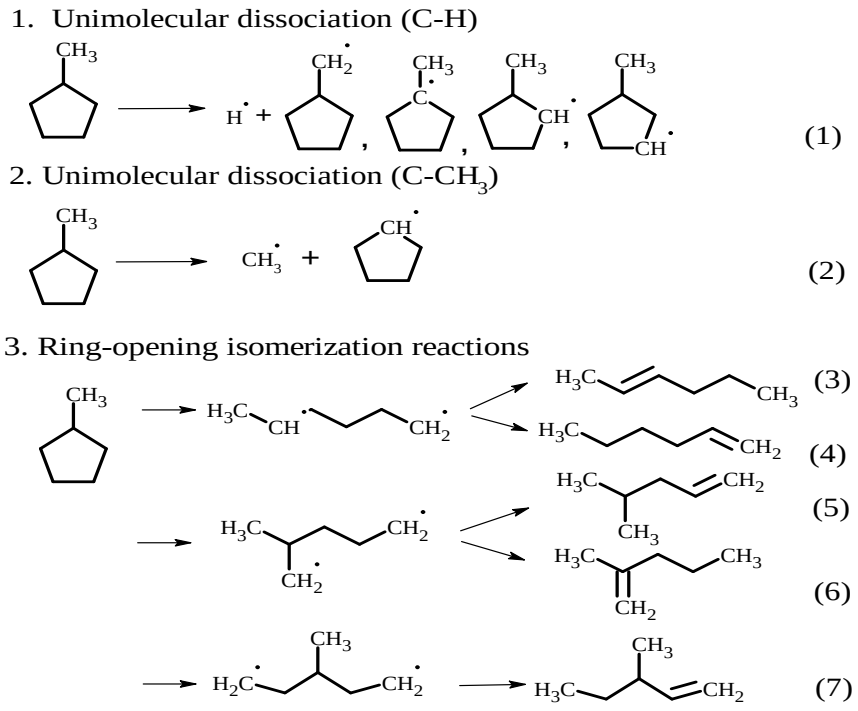


Figure 5.1: Scheme for unimolecular decomposition and ring-opening isomerization of MCP.

isomers, as shown in Figures 5.1 and 5.2. The competition between the last two steps has a significant impact on the overall decomposition mechanism and the production of aromatic compounds.

The study includes:

- The pyrolysis experiment of MCP was performed in a single-pulse shock tube (CST facility) at elevated pressure and temperature conditions (specify T and P). GC-FID/FID and GC-MS have been employed for the detection, identification, and quantification of the detected products.
- This work conducts a detailed investigation of the chemical pathways involved in MCP pyrolysis using quantum chemistry methods, incorporating single-reference and multireference calculations as necessary. In our theoretical calculations, we also examine ECP for the comparison of the initial dissociation channels of alkylated cyclopentane. Further, this study

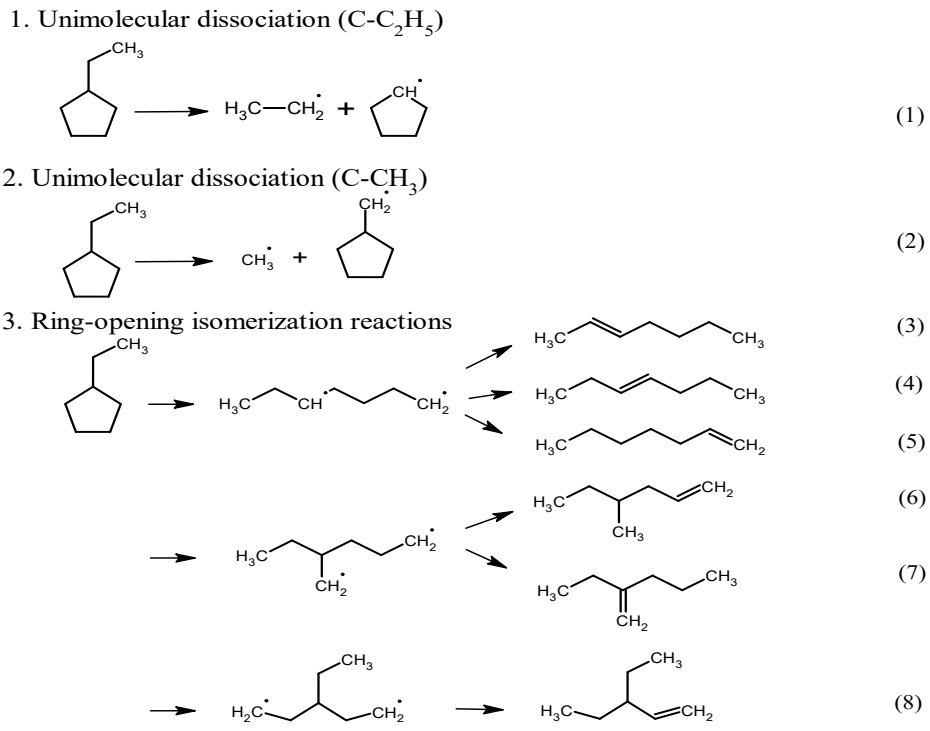


Figure 5.2: Scheme for unimolecular decomposition and ring-opening isomerization of ECP.

presents an in-depth investigation of the unimolecular dissociation (loss of -H, -CH_3, -C_2H_5 groups) and ring isomerization pathways of MCP and ECP using high-level ab initio calculations (multireference calculations). The reaction rates were determined based on the calculated potential energy surfaces using transition state theory (TST) and variational transition state theory (VTST) across a wide temperature range of 800-2000 K.

- Finally, a detailed combined chemical kinetic model for the pyrolysis and oxidation of CPT, MCP, and ECP was established. The method was built on the prior models of CPT and MCP. The model was revised for the MCP rate constants calculated in the thesis chapter. For ECP, all the rate constants were computed using procedures similar to those employed for MCP. For all remaining reactions involving ECP, the rate constants are derived from the rate constants of MCP and CPT. The newly developed model was validated using more experimental measurements of MCP py-

rolysis. Currently, there are no shock tube data available for validation in ECP studies.

- The ROP and sensitivity analysis of MCP under pyrolysis conditions have been investigated, with an emphasis on the unimolecular dissociation/initial decomposition stages of MCP, as well as the formation of toluene and benzene, as derived from kinetic simulations.

This thesis chapter is structured in the following manner: Section 5.2 describes the experimental methods used to investigate the thermal decomposition of methyl cyclopentane. Section 5.3 describes the computational methodology used to investigate the thermal decomposition of MCP. The section includes details of the quantum chemistry methods used for geometry optimization, frequency calculations, and reaction rate calculations. The results of the theoretical calculations are discussed in Section 5.4. The section includes the potential energy surface diagrams and considers the reaction mechanisms involved. Furthermore, the high-pressure limit (HPL) rate constants, computed based on quantum chemistry calculations for a temperature range of 800–2000 K, are discussed. Section 5.5 discusses the pyrolysis experiments and kinetic simulations. The identified chemical routes from GC results are employed in ANSYS Chemkin, and the resultant products are simulated throughout a temperature range for comparison with experimental data on MCP pyrolysis. This section also analyzes the ROP and sensitivity of MCP during pyrolysis conditions. Section 5.6 is the conclusion part of our study. In conclusion, the study's main findings are presented.

5.2 Experimental methods

The thermal decomposition of MCP was studied in the Chemical Shock Tube facility (CST-1). The specifications of the shock tube equipment have been established in an earlier chapter. This section gives some essential features. The CST comprises an aluminum tube with a 50 mm internal diameter and 25 mm wall thickness. The length of the driver section is 1.8 m, and that of the driven section side is 3.3 m. The pneumatic ball valve is positioned in the driven section, 0.4 m from the end flange, which is referred to as the sample chamber or reaction chamber. Although this method was introduced by Tschuikow-Roux in 1970 [189], it has recently been referred to as the constrained reaction volume strategy by Hanson's group [255]. The experiment utilized an aluminum diaphragm with a thickness of 1-2 mm and variable grooving for bursting.

The time intervals between the rising fronts of the pressure trace from the incident shock are utilized to calculate the incident shock velocity and Mach number. The actual T_5 temperature has been calculated with a correlation between T_5(theoretical) and T_5(kin) using an external chemical thermometry method. The T_5 (theoretical) temperature behind the reflected shock waves was calculated from the incident shock velocity using the standard one-dimensional normal shock equations from the Wisconsin Gas Dynamics Calculator [256]. T_5 (kin) was determined utilizing the previously known rate constants of ethyl chloride and 1,1,1-trifluoroethane as external chemical thermometers within the temperature ranges of 960–1300 K and 1300–1500 K, respectively, as described in Chapter 02.

A mixture of MCP (vapor pressure of 233 mmHg at 35°C) ($\geq$98% purity, TCI (Tokyo Chemical Industry)) and argon (99.999% purity) was prepared in

the SS mixing tank. The quantification and identification of the pre-shock and post-shock gas mixtures were performed utilizing a gas chromatograph with a dual flame ionization detector (GC-FID/FID, Agilent 7890B) and a gas chromatograph coupled with a quadrupole mass detector (GC-MS, Agilent 7890A). The quantification of light hydrocarbons (C_5) has been achieved using front-FID with an HP-PlotQ column, whereas higher hydrocarbons (C_5 and above) were quantified using back-FID coupled to an HP-5 column. GC-MS with a DB-1 column has been employed to identify hydrocarbons with m/z>42. The FIDs of the gas chromatograph have been calibrated with hydrocarbons, utilizing known quantities of reference gases. The calibration procedure has yielded an estimated error of 5%.

5.3 Computational methods

Ab initio simulations are helpful in explaining the potential energy surface (PES) associated with unimolecular decomposition. CASSCF/MRCI (multireference) [191, 192], and CBS-QB3 (single reference) [193] methods have been used for the calculations. The geometry optimizations and frequency calculations were performed utilizing the CASSCF method (zero-point energy (ZPE) scale factor is 0.93) together with the 6-31+g(d,p) basis set for multireference calculations. The geometry optimizations and frequency calculations were performed utilizing the CASSCF method (zero-point energy (ZPE) scale factor is 0.93) together with the 6-31+g(d,p) basis set for multireference calculations. MCP and ECP contain 24 and 28 doubly occupied molecular orbitals, respectively. Consequently, the active orbitals in CAS(6e, 6o) correspond to orbital numbers 22-27 (MCP) and 26-31 (ECP), and CAS(2e, 2o) corresponds to orbital numbers 24-25 (MCP) and 28-29 (ECP). In the context of C-H, C-CH_3,

and C-C_2H_5 dissociation (unimolecular decomposition), the active space involves two electrons occupying two orbitals, denoted as CAS (2e, 2o), and for the C-C bond dissociation (ring opening), it is (6e, 6o). Corrections to single-point energies have been done by the MRCI method with the same active space and basis set. The CBS-QB3 approach was used to calculate the H-abstraction and methylcyclopentyl radical decomposition pathways. This method involves several steps, starting with a geometry optimization at the B3LYP/6-311G (2d, d, p) level (with a ZPE scale factor of 0.99) and followed by a high-level single-point energy calculation, which includes complete basis set extrapolation. Transition structures (TS) were determined based on the presence of a single imaginary frequency in the normal mode coordinate analysis. Intrinsic Reaction Coordinate (IRC) calculations conducted in both directions, starting from the optimized transition state structure, verify the saddle points as the correct ones connecting the reactant(s) and product(s) for the given reaction. Multireference calculations were performed by the Molpro package [258], and the rest of the single-reference calculations were performed by the Gaussian 16 [197] program.

High-pressure limit rate constants for all elementary reactions having a saddle point were computed using conventional transition state theory (TST).

$$k(T) = \sigma \frac{k_B T}{h} \frac{Q_{\neq}}{\Pi Q_R} exp(-\frac{\Delta E_0}{RT})$$

where σ is the symmetry number, k_B is the Boltzmann constant, h is the Planck's constant, T is the temperature, Q_R is the total molar partition function for reactants (consisting of the translation, vibration, rotation, and hindered rotation), $Q_{\neq}$ is the partition function of the activated complex, and ΔE_0 is the electronic energy barrier, including ZPE. The loss of the CH_3 channel

does not have a barrier and hence requires a variational treatment.In Variational Transition State Theory (VTST), the rate is calculated by minimizing the generalized transition state theory (TST) rate constant, k(s,T), with respect to the position of the dividing surface (reaction coordinate), (s). The temperature (T) is a parameter used to calculate the rate constant.

$$k_{VTST} = min k_{TST}(s, T)$$

where (s) is the location of the dividing surface along the reaction coordinate and $k_{TST}(s, T)$ represents the rate constant at each point along the reaction coordinate. In most cases, internal degrees of freedom were regarded as rigid rotor harmonic oscillators. It is important to emphasize that the restricted rotations of the cyclic structure were also considered harmonic oscillators, which also included flexible movements of the ring. On the other hand, the unrestricted alkyl groups (e.g., internal rotation of the methyl group) were viewed as one-dimensional hindered internal rotors. The internal rotors were considered using the hindered rotor feature of the Gaussian 16 program [197], with the hindrance potentials calculated at the B3LYP/6-311G (2d, d, p) level. The potential energy for each internal rotation of the reactant was calculated by performing a relaxed energy scan of the dihedral angle at 10-degree intervals (36 steps for 360 degrees). For the transition state, the potentials of hindered internal rotations, which are nearest to the reaction sites, were calculated with the bond lengths at the critical geometries held constant (using the bond freeze option in Gaussian 16).

To implement chemical kinetic modeling effectively, three kinetic parameters, A, n, and E_A are determined by fitting the calculated rate constants across a temperature range of 800-2000 K in increments of 50 K to a modified

Arrhenius equation. Given that we achieved a reasonable correlation with the temperature coefficient, giving a value of n = 0 within the examined temperature range, we opted to leave the temperature coefficient at zero. The revised Arrhenius equation for n=0 is presented below.

$$k(T) = Aexp(-\frac{\Delta E_a}{RT})$$

The rate constant computations were conducted using the Multiwell 2023 program package [260]. The thermal module of the multiwell was utilized for transition-state theory (TST) calculations, while the ktools module was employed for variational transition-state theory (VTST) calculations.

5.4 Results and Discussion

The starting point for the thermal decomposition of MCP and ECP, as well as the subsequent reactions, can be categorized into the following steps. Our calculations commence with the lowest-energy conformer of MCP and ECP, as determined by CBS-QB3 calculations.

1. Unimolecular decomposition and ring-opening isomerization of MCP and ECP: The reaction involves the dissociation of the C-CH_3, C-C_2H_5, and C-H bonds, resulting in the formation of a cyclopentyl and methylcyclopentyl radical. Ring-opening of the cyclopentane group produces five alkenes via three distinct biradical intermediates.

2. H-abstraction reaction of MCP and ECP: The chain reactions occur via the H-abstraction from different carbon atom sites of MCP and ECP by hydroxyl radical (OH), hydrogen atom (H), oxygen atom (O), methyl

radical (CH_3), and hydroperoxyl radical (HO_2). The H-abstraction results in four types of methylcyclopentyl and five ethylcyclopentyl radicals.

3. Decomposition and isomerization of methyl cyclopentyl and ethylcyclopentyl radicals: Methylcyclopentyl or ethylcyclopentyl radicals can either isomerize to generate alkenyl radicals or produce cyclic intermediates or aromatics through stepwise dehydrogenation. The alkenes and alkenyl radicals further undergo decomposition into smaller fragments and radicals as secondary reactions.

The subsequent two sections discuss the potential energy surface (PES), which includes the reaction mechanisms for all the classes of reactions mentioned so far. Following the PES section, the discussion focuses on the thermal rate constants associated with each of the involved reactions.

5.4.1 Unimolecular decomposition and ring-opening isomerization

All the possible reaction channels of the initial unimolecular decomposition and isomerization pathways of MCP are shown in Figure 5.1. In this process for MCP, cyclopentyl and methylcyclopentyl radicals, two hexenes (through biradical intermediate 1), and three methylpentenes (through biradical intermediates 2 and 3) are produced. In this process for ECP, cyclopentyl and methylcyclopentyl radicals, three heptenes (through biradical intermediate 1), and methylhexenesxene and ethylpentene (through biradical intermediates 2 and 3) are produced.

Barrierless bond fission reactions demonstrate significant multireference characteristics when the chemical bond is elongated. Thus, for the unimolecular

decomposition pathways of methyl and ethyl elimination, we have considered two active space orbitals corresponding to the C-C bonding orbital and C–C antibonding orbital. Also, the minimum energy potentials (MEPs) for these reactions were determined by conducting a relaxed scan along the reaction coordinates by incrementally increasing the step size to 0.1 Å in the MRCI//CASSCF method (Figure 5.3). Figures 5.4 and 5.5 represent the calculated potential

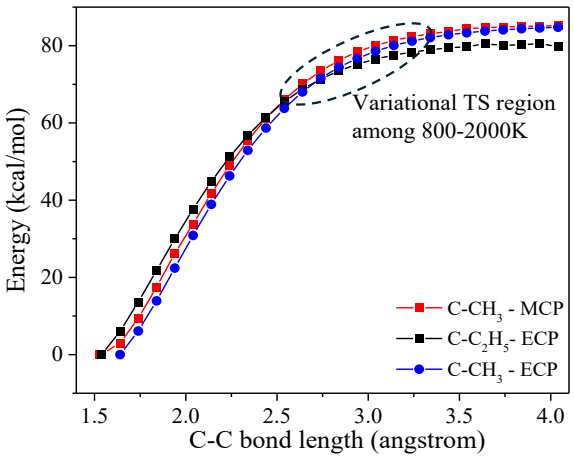


Figure 5.3: Stepwise optimized potential energy curve of methyl and ethyl loss from MCP and ECP at MRCI/6–31+g(d,p)//CAS(2,2)/ 6–31+g(d,p). Energy unit: kcal/mol

energy surfaces for all the mentioned reaction channels. The bond dissociation energy (BDE) for C-H bond cleavage is significantly higher than that for C-C bond cleavage, with a difference above 10 kcal/mol for MCP (not calculated for ECP, as C-H scission would be similar). Consequently, the initial cleavage of the C-C bond occurs more rapidly than that of the C-H bond. The PES indicates that the initial decomposition pathway of -CH_3, -C_2H_5 loss has a lower energy barrier than the C-C ring opening isomerization pathways. The formation of the methyl and the cyclopentyl radical (for MCP) and the ethyl and cyclopentyl radical (for ECP) is the most preferred reaction.

Ring-opening isomerization happens in two steps. Initially, the cyclopentane ring undergoes C-C bond dissociation, resulting in three biradical intermediates

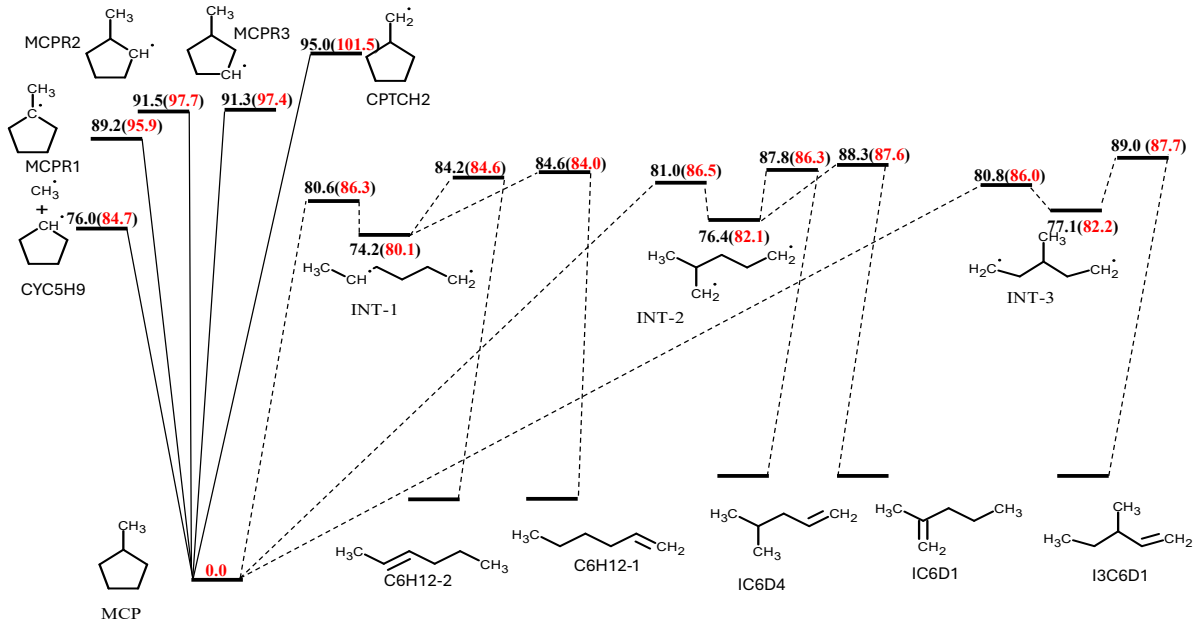


Figure 5.4: Potential energy surface for unimolecular decomposition (C-CH_3, C1-H, C2-H, C3-H, and C4-H bond dissociation) and ring-opening isomerization (C2-C3, C3-C4, and C4- C5 bond dissociation) of MCP. For the unimolecular decomposition, the methods MRCI/6–31+g(d,p)//CAS(2,2)/6–31+g(d,p) (value in the bracket with red color) and CAS(2,2)/ 6–31+g(d,p) (value with black color) were used. For isomerization, the methods MRCI/6–31+g(d,p)//CAS(6,6)/6–31+g(d,p) (value in the bracket with red color) and CAS(6,6)/6–31+g(d,p) (value with black color) were used. Energy unit: kcal/mol

for both MCP and ECP. The second step is H-migration, which results in the formation of alkenes. There are three different ring C-C bonds in MCP and ECP: C1–C2, C2–C3, and C3–C4. The opening of the ring creates three biradical intermediates. The energy barrier for all three biradical intermediates is similar in magnitude, considering the MRCI energies (within 0.5 kcal/mol).

Table 5.1 presents a comparison of the energy barriers associated with the isomerization and the unimolecular decomposition pathways of cyclopentane (CPT), methylcyclopentane (MCP), cyclohexane (CH), methylcyclohexane (MCH), and isopropylcyclohexane (IPCH). The table indicates that the C-H bond dissociation energy is the highest among all the steps. The initial decomposition channel producing the CH_3, $C_{2,5}$ and C_3H_7 radicals has a lower energy barrier than the ring-opening reactions for MCP, MCH, and their alky-

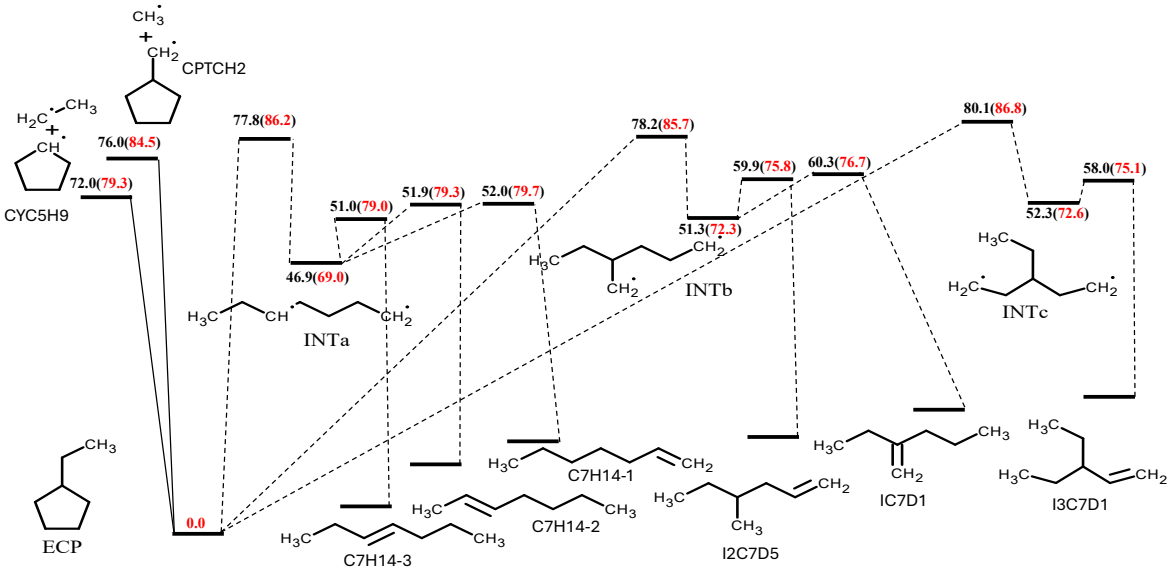


Figure 5.5: Potential energy surface for unimolecular decomposition (C-C_2H_5, C-CH_3 bond dissociation) and ring-opening isomerization (C2-C3, C3-C4, and C4-C5 bond dissociation of ECP). For the unimolecular decomposition, the methods MRCI/6–31+g(d,p)//CAS(2,2)/6–31+g(d,p) (value in the bracket with red color) and CAS(2,2)/ 6–31+g(d,p) (value with black color) were used. For the ring-opening isomerization, the methods MRCI/6–31+g(d,p)//CAS(6,6)/6–31+g(d,p) (value in the bracket with red color) and CAS(6,6)/6–31+g(d,p) (value with black color) were used. Energy unit: kcal/mol

Table 5.1: Comparison of unimolecular decomposition and ring-opening isomerization reactions of cyclohexane and cyclopentane and their alkylated derivatives. Energy unit: kcal/mol

	CH[a]	MCH[b]	IPCH[c]	CPT[d]	MCP[e]	ECP[f]
H elimination	97.8	98.9/93.5/96.9/96.7/96.7	-	97.5	101.5/95.9/97.7/97.4	-
CH_3 elimination	-	84.0	83.2	-	84.7	84.5
C_2H_5 elimination						79.3
C_3H_7 elimination	-	-	81.6	-	-	-
TS of C1-C2	88.7	85.0	85.9	85.9	86.3	86.2
TS of C2-C3	-	89.0	88.0	-	86.5	86.7
TS of C3-C4	-	89.0	87.6	-	86.0	86.3

[a] CASPT2/cc-pVDZ [259] [b] CASPT2/cc-pVDZ [261] [c] MRCI [130]. [d,e,f] MRCI (This work).

lated derivatives. The alkylated cycloalkanes start dissociating faster than the cycloalkanes (for example, MCP will dissociate faster than CPT). The reactivity among cyclopentane derivatives is as follows: ECP > , MCP > , CPT. It is also interesting to note that the C1-C2 bond dissociation energy (adjacent to the alkyl (methyl, ethyl) groups) is the lowest among the ring-opening isomerization pathways (more evident in cyclohexanes compared to cyclopentane). These observations clearly show the effect of the alkyl group on the reactivity of cycloalkanes.

In the second step, the biradicals undergo intramolecular H-migration, in which a radical abstracts a hydrogen atom from a carbon atom adjacent to the second radical. These reactions result in the formation of five alkene isomers. Intramolecular H-migration energy barriers are almost similar due to similar cyclic transition states. Table 5.2 shows the details of the different cases of H migration in the second step of ring opening of methylcyclopentane. H migration barriers for MCP and ECP are comparable due to similar cyclic transition states.

5.4.2 H-abstraction reaction by H atom and CH_3 radical

The CBS-QB3 level of theory was used for all the abstraction reactions. Geometry optimization and vibrational frequency were carried out at the B3LYP/6-

Table 5.2: H-migration TS energy barriers. Methods: MRCI//CAS(6,6)/6-31+g(d,p) Energy unit: kcal/mol.

H-migration details	TS barrier (kcal/mol)
Cyclic TS states	
INT1 = C6H12-1	3.9
INT1 = C6H12-2	4.5
INT2 = IC6D4	4.2
INT2 = IC6D1	5.5
INT3 = I3C6D1	5.5

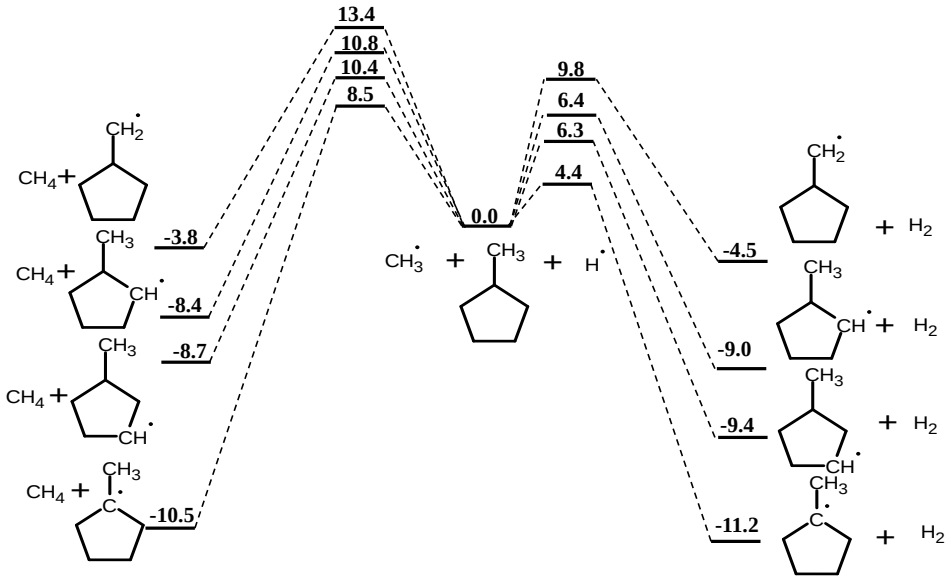


Figure 5.6: Potential energy surface for H-atom abstraction reactions of MCP by H atom and CH_3 radical. Energy unit: kcal/mol.

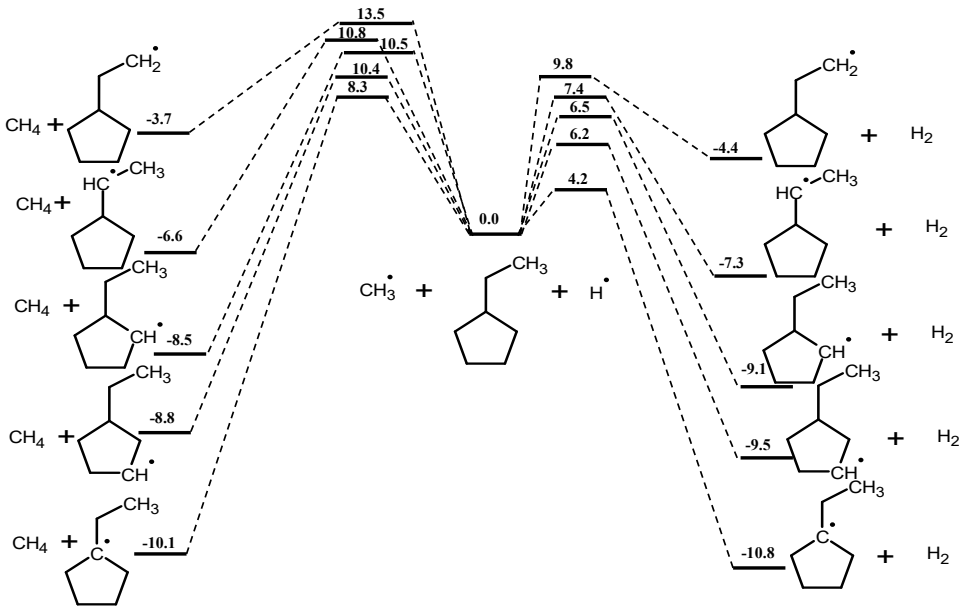


Figure 5.7: Potential energy surface for H-atom abstraction reactions of ECP by H atom and CH_3 radical. Energy unit: kcal/mol.

311G (2d,d,p) level. Figures 5.6 and 5.7 illustrate the potential energy surface for all the possible reaction paths. MCP contains four distinct carbon atoms, leading to the formation of four distinct methylcyclopentyl radicals. The ECP contains five distinct carbon atoms, leading to the formation of five distinct ethylcyclopentyl radicals.

The energy barrier for hydrogen abstraction by a hydrogen atom is lower than that for hydrogen abstraction by a methyl radical. Table 5.3 shows a comparison between the H-abstraction of MCP and ECP. The positions of hydrogen atoms (primary, secondary, and tertiary) and the bond dissociation energies (BDEs) of carbon-hydrogen (C-H) bonds significantly influence hydrogen abstraction reactions for all molecules. The PES and the table for H-abstraction also show the energy barrier for the primary carbon (PX) $>$, secondary carbon (SX) $>$ tertiary carbon (TX) in both MCP and ECP radicals. The energy barriers for abstraction reactions are lower than those for unimolecular reactions and alkylcyclopentane decomposition reactions. Hydrogen abstraction reactions primarily produce hydrogen and methane.

Table 5.3: Comparison of the transition state energy barrier of the H-abstraction reaction by the H atom between MCP and ECP. Energy unit: kcal/mol. Method: CBS-QB3

H-abstraction	MCP	ECP
Side chain		
C1-P1X	9.8	9.8
C2-S2X	-	7.2
CPT ring		
C1 -TX	4.4	4.2
C2 -S2X	6.4	6.5
C3 -S3X	6.3	6.2

5.4.3 Decomposition and isomerization of methyl cyclopentyl and ethyl cyclopentyl radicals

The hydrogen atom abstraction of MCP and ECP results in methyl cyclopentyl and ethyl cyclopentyl radicals, as illustrated in Figures 5.6 and 5.7. Figures 5.8 and 5.10 show possible unimolecular dissociation reactions of methylcyclopentyl and ethylcyclopentyl radicals that proceed either by β-C-H scission, β-C-C scission eliminating methyl or ethyl group, or by the ring opening isomerization via β-C-C scission, leading to the opening of the five-membered ring. The ring-opening isomerization pathways, which involve the cleavage of the C-C bond nearest to the side chain, have a lower energy barrier. This trend is similar to that of alkylated cyclohexanes, such as MCH, ECH, and IPCH. The dissociation that leads to the methyl group and cyclopentene had a slightly lower energy barrier than the ring-opening isomerization pathways. The energy barrier for dissociation through the β-C-H scission was higher in almost all cases.

The C_6 and C_7 chains generated from the decomposition of MCP and ECP radicals subsequently decompose into smaller components via β-C-C scission (see figure 5.9 and 5.11).

From the PES diagram of MCP and ECP, it can be concluded that the initial decomposition channels (side chain dissociation) are the most important

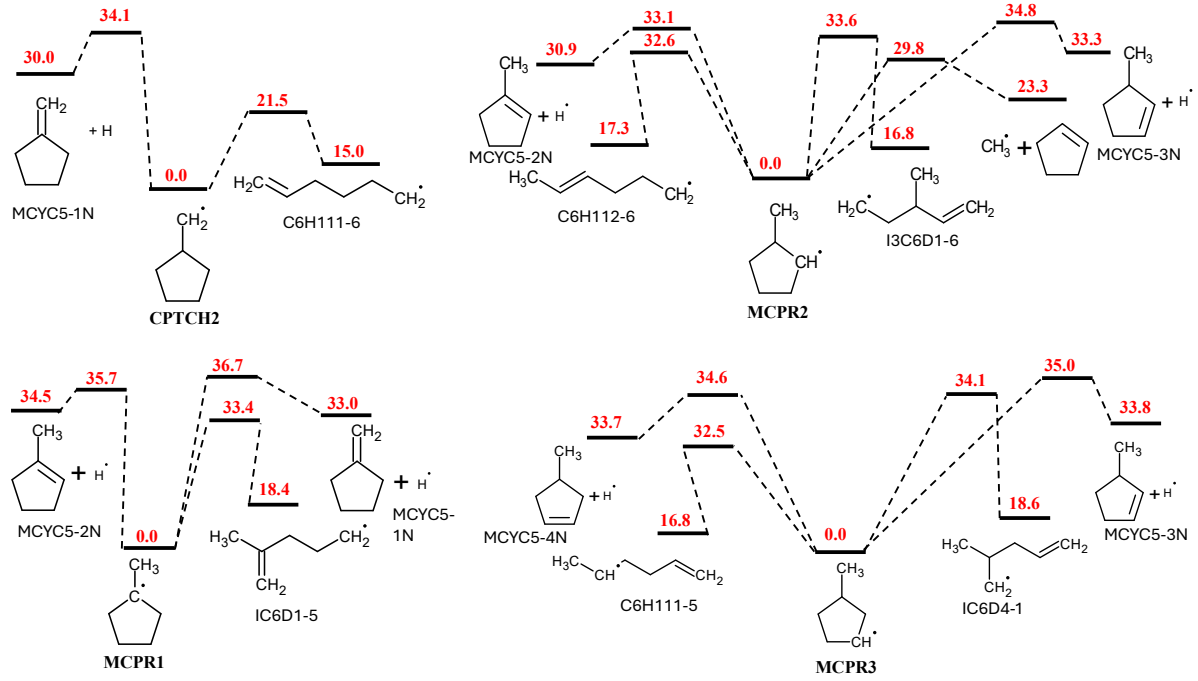


Figure 5.8: Potential energy surface for the decomposition of MCP radicals. For the decomposition, the methods CBS-QB3//B3LYP/6–311G(2d,d,p) were used. Energy unit: kcal/mol

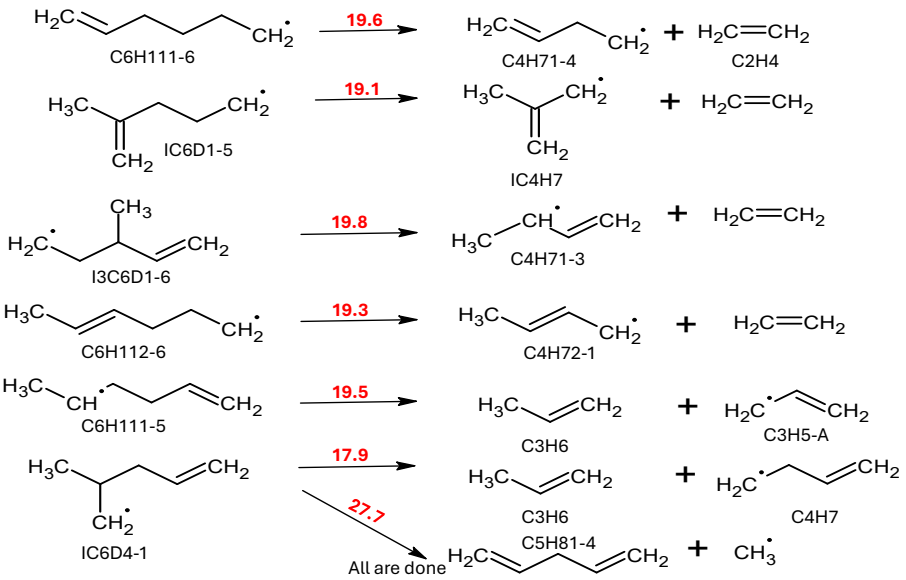


Figure 5.9: Decomposition of the hexane radicals for MCP

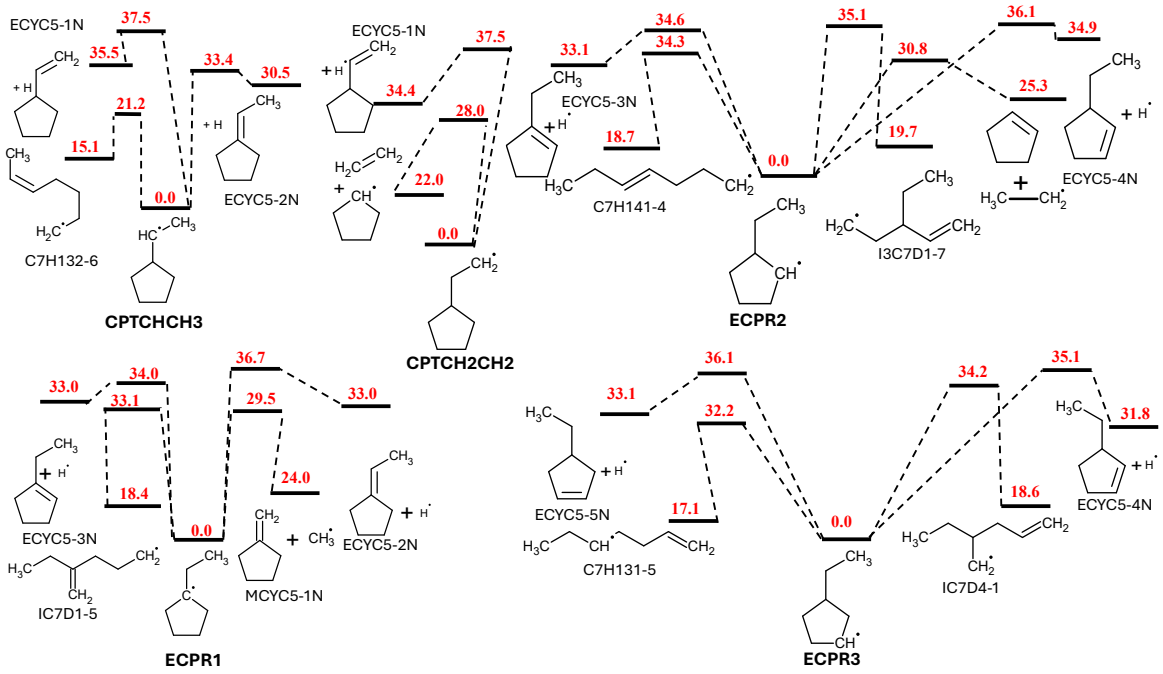


Figure 5.10: Potential energy surface for the decomposition of ECP radicals. For the decomposition, the methods CBS-QB3//B3LYP/6–311G(2d,d,p) were used. Energy unit: kcal/mol

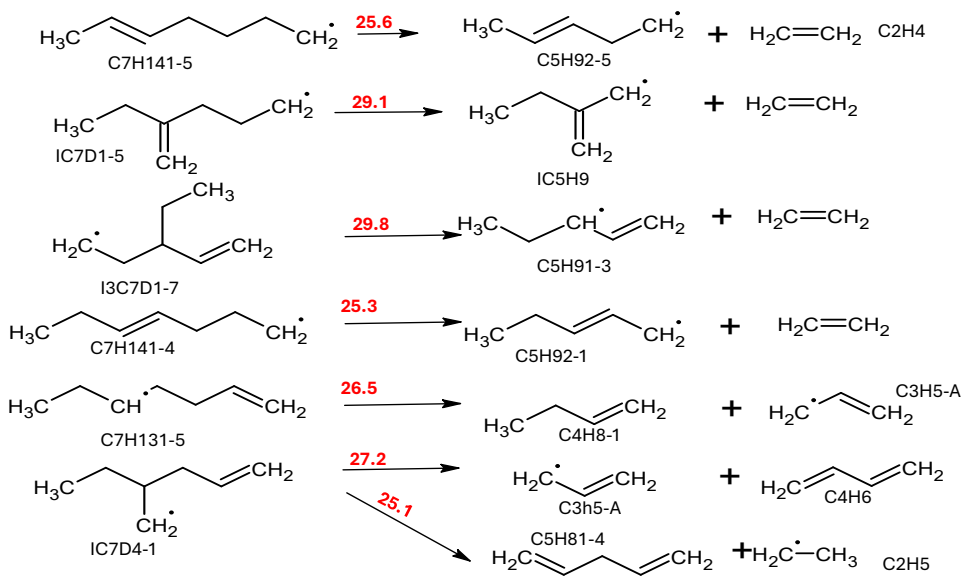


Figure 5.11: Decomposition of the heptane radicals for ECP

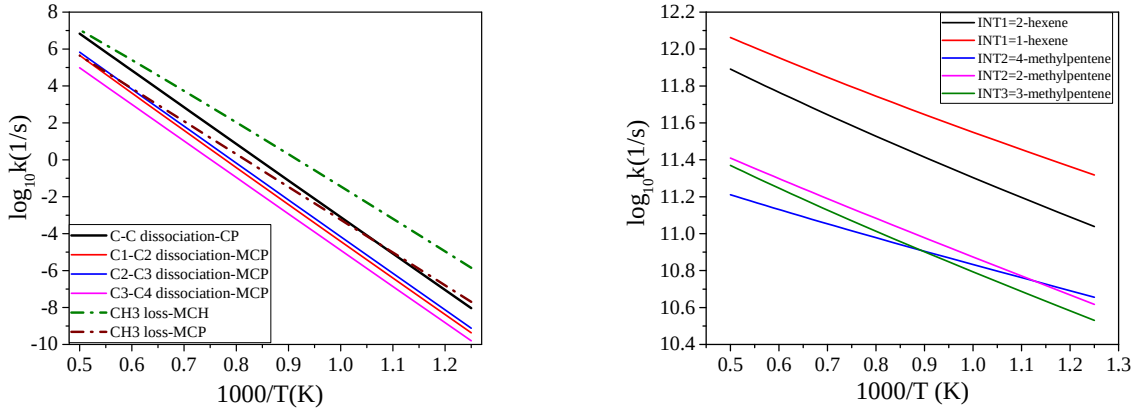
reaction step for alkylated cyclopentanes. The following steps, including the ring-opening reactions, abstraction reactions, and alkyl cyclopentyl decomposition, exhibit comparable activation energies, indicating that monoalkylated cyclopentanes follow analogous decomposition pathways. This is important since one can employ the computed rates from MCP for the rate calculations of ECP, IPCP, and other alkylated cyclopentanes.

5.4.4 Rate constant calculations

The high-pressure limit (HPL) temperature-dependent rate constants were determined using conventional transition state theory (TST) for reactions with a saddle point and variational transition state theory (VTST) for barrierless reactions (no saddle point) within the temperature range of 800–2000 K. Tables 5.4 and 5.5 show the rate constants of the decomposition channels of methyl cyclopentane: unimolecular decomposition, ring-opening isomerization, abstraction reactions of MCP, and subsequent radical decomposition. The focus of this chapter is exclusively on the rate constants for MCP, as the aim is to validate MCP shock tube speciation results.

Unimolecular decomposition and ring-opening isomerization of MCP

According to the calculations on MCP/MCH, the bond dissociation energy for the C-H bond is much higher than that for ring-opening isomerization reactions. Hence, rate calculations for C-H scission are not compared to the initial reaction channels. It is important to compare the HPL rate constants of the methyl loss channel and the ring-opening isomerization reaction, MCP. The step-by-step, optimized potential energy curve for the dissociation of MCP through methyl loss is shown in Figure 5.3. The barrier height of variational



(a) (b)

Figure 5.12: Rate constants for unimolecular dissociation and ring-opening isomerization of MCP; (*a*) Comparison of the rate constant of the unimolecular decomposition (MCP and MCH) and ring-opening isomerization reaction (CPT and MCP); (*b*) H migration rate constants of MCP.

transition states ranged from 66 to 83 kcal/mol at temperatures between 800 and 2000 K, while the C-C bond stretching varied from 2.5 to 3.3 Å. Therefore, it is important to compare the energies of the variational transition state for the methyl elimination pathways and those of the ring-opening isomerization. Figure 5.12 shows a comparison between the rate constants of the unimolecular decomposition (MCP and MCH) and the ring-opening isomerization reaction (CP and MCP). The methyl loss channel is the most important reaction among the initial reactions in MCP and MCH (methyl loss in MCH has a higher rate constant with a lower energy barrier than MCP). However, with the temperature rise, the rate constants are similar to the C-C bond dissociation channels because the A-factor of isomerization reactions is higher.

Figure 5.12 shows the HPL rate constants of the ring-opening isomerization (2nd step) of MCP (intramolecular H-migration from biradical to form alkenes). The rates for the intramolecular H-migration step are significantly higher than those for the first step, primarily due to lower energy barriers (biradical intermediates are highly reactive).

H-abstraction reaction by H atom and CH_3 radical

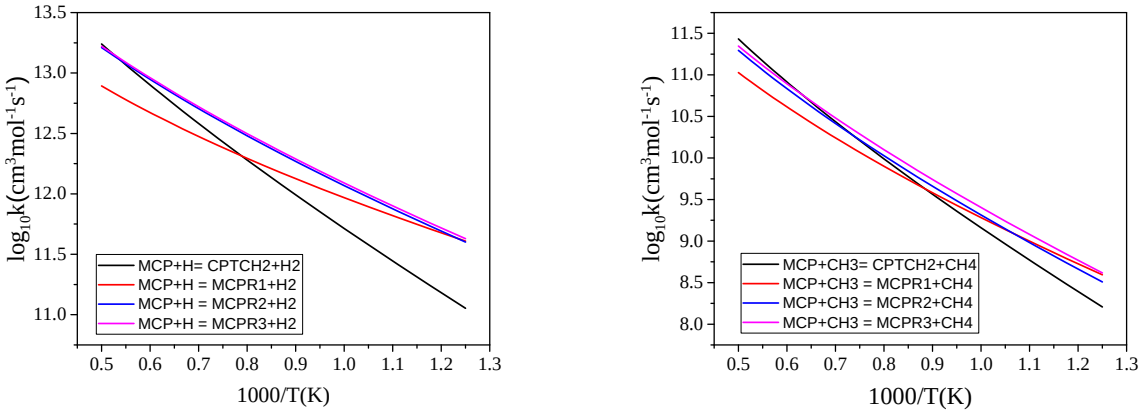


Figure 5.13: HPL thermal rate constant of H-abstraction reactions of MCP by H -atom and CH_3 radical.

Figure 5.13 presents the rate constants of H-abstraction reactions of MCP H-atom and CH_3 radical. Abstraction reactions significantly influence MCP consumption owing to minimal energy barriers. The rate constants for S3X and S4X carbon are almost identical due to similar activation energies. The rate constants exhibit distinct differences, with H-abstraction rates with H atoms being lower than those of methyl radicals. The abstraction processes were estimated for the O, OH, and HO_2radicals to compare oxidation reactions from previous investigations.

Table 5.4: High-pressure limit (HPL) rate constants of the primary decomposition channels of methyl cyclopentane: unimolecular decomposition, ring-opening isomerization, and abstraction reactions of MCP.

SN	Reaction	A (s^{-1})	Ea (cal/mol)
	Unimolecular decomposition		
1	MCP = cC5H9+CH3	3.40E+15	81331.9
2	MCP = INT1	4.43E+15	91764.9
3	MCP = INT2	6.11E+15	91248.2
4	MCP = INT3	6.81E+14	90258.6
5	INT1 = C6H12-1	2.83E+12	5236.5
6	INT1 = C6H12-2	1.78E+12	4573.5
7	INT2 = IC6D4	3.76E+11	3392.9
8	INT2 = IC6D1	8.57E+11	4841.6
9	INT3 = I3C6D1	8.33E+11	5144.3
	Abstraction reaction		
10	MCP+CH3= CPTCH2+CH4	3.26E+13	19829.5
11	MCP+CH3 = MCPR2+CH4	1.21E+13	17161.5
12	MCP+CH3 = MCPR3+CH4	1.25E+13	16810.7
13	MCP+CH3 = MCPR1+CH4	3.80E+12	15000.0
14	MCP+H= CPTCH2+H2	4.59E+14	13436.9
15	MCP+H = MCPR2+H2	1.76E+14	10214.6
16	MCP+H = MCPR3+H2	1.66E+14	9863.3
17	MCP+H = MCPR1+H2	5.14E+13	7921.4
18	MCP+O= CPTCH2+OH	2.61E+14	9890.5
19	MCP+O = MCPR2+OH	1.79E+14	7603.8
20	MCP+O = MCPR3+OH	1.56E+14	7248.3
21	MCP+O = MCPR1+OH	2.68E+13	5727.1
22	MCP+OH= CPTCH2+H2O	1.82E+09	5766.7
23	MCP+OH = MCPR2+H2O	4.51E+09	5201.1
24	MCP+OH = MCPR3+H2O	2.29E+09	4619.8
25	MCP+OH = MCPR1+H2O	1.43E+09	3449.6
26	MCP+O2H= CPTCH2+H2O2	5.74E+13	24627.4
27	MCP+O2H = MCPR2+H2O2	1.51E+13	20655.0
28	MCP+O2H = MCPR3+H2O2	1.98E+13	20446.3
29	MCP+O2H = MCPR1+H2O2	2.95E+12	17479.4

Table 5.5: High-pressure limit (HPL) rate constants of the decomposition channels of methyl cyclopentane radicals.

SN	Reaction	A (s^{-1})	Ea (cal/mol)
1	CPTCH2=MCYC5-1N+H	2.50E+12	36843.0
2	CPTCH2=C6H111-6	1.51E+12	23381.1
3	MCPR2=IC5D1-6	3.44E+12	34569.8
4	MCPR2=MCYC5-3N+H	4.13E+14	37689.4
5	MCPR2=C6H111-5	7.78E+13	34571.8
6	MCPR2=CYC5H8+CH3	3.81E+14	32441.7
7	MCPR2=MCYC5-2N+H	1.39E+13	34965.2
8	MCPR1=MCYC5-2N+H	7.78E+17	41337.5
9	MCPR1=IC6D1-5	3.03E+16	38494.2
10	MCPR1=MCYC5-1N+H	4.91E+16	40290.4
11	MCPR3=MCYC5-3N+H	2.06E+14	37500.7
12	MCPR3=C6H111-5	6.34E+13	34238.0
13	MCPR3=MCYC5-4N	4.14E+15	37858.3
14	MCPR3=IC6D4-1	9.89E+12	35078.5

5.5 Experiment and simulation

In pyrolysis investigations performed at temperatures ranging from 950 to 1600 K and pressures between 10 and 25 bar, a total of 15 species were identified, as shown in Figs. 5.14 and 5.15. C1–C5 species that are detected are methane (CH_4), acetylene (C_2H_2), ethylene (C_2H_4), ethane (C_2H_6), allene (C_3H_4-A), propene (C_3H_6), propyne (C_3H_4-P) 1,3-butadiene (C_4H_6), but-1-ene (C_4H_8), vinylacetylene (C_4H_4), 1,3-butadiyne (C_4H_2), cyclopentene (cC_5H_8), and cyclopentadiene (C_5H_6). Benzene (C_6H_6) and toluene ($C_6H_5CH_3$) are the aromatic compounds detected during the experiment.

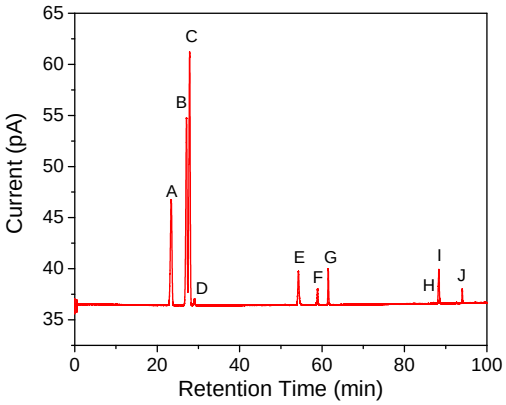


Figure 5.14: GC Chromatogram at 1520 K from front-FID (lower boiler species). Peaks are assigned to (A) methane, (B) ethylene, (C) acetylene, (D) ethane, (E) propene, (F) allene, (G) propyne, (H) vinylacetylene, (I) 1,3-butadiene, (J) 1,3-butadiyne (C_4H_2)

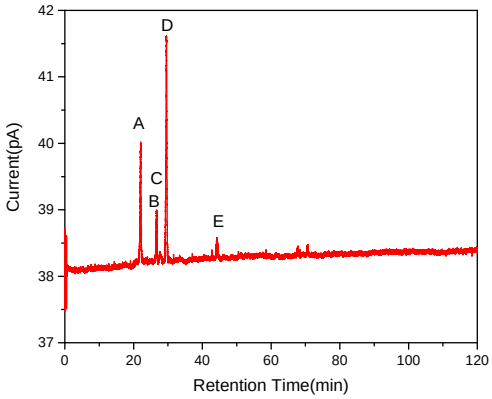


Figure 5.15: GC chromatogram at 1520 K from back-FID (higher boiler species). Peaks are assigned to A=cyclopentadiene, B=methyl cyclopentane, C=cyclopentene, D=benzene, and E=toluene.

The carbon balance method is used to calculate the initial reaction concentration based on the hypothesis that all carbon remains in the gas phase, as indicated in the preceding study [257]. Using the carbon balance method,

$$[MCP]_0 = [MCP]_t + \sum_{i=1}^{15} \frac{n_i[P_i]_t}{6}$$

In this equation, $[MCP]_0$ denotes the initial concentration of methyl cyclopentane, $[MCP]_t$ indicates the concentration of methyl cyclopentane at time t, n_i

represents the number of carbon atoms in the i^{th} product, and $[P_i]_t$ signifies the concentration of the i^{th} product at time t.

The distributions of the normalized concentrations of reactants and all products, including both minor and major species, within the experimental temperature range, as determined by kinetic modeling, are presented and analyzed in the following sections. To gain insight into the chemistry governing the decomposition of MCP and the formation of aromatic chemicals, rate of production (ROP) analysis and sensitivity analysis were conducted at different conditions.

5.5.1 Primary decomposition of MCP

Figures 5.16, 5.19 , and 5.20 depict the experimental and simulated mole fraction distributions of MCP. The current model accurately forecasts general trends in MCP decomposition in relation to temperature. MCP begins to degrade at approximately 1150 K and is entirely consumed at temperatures beyond 1500 K. Figure 5.17 illustrates the principal mechanisms of MCP decomposition, including unimolecular dissociation, ring opening, and hydrogen abstraction processes predominantly involving H and CH_3 radicals. Unimolecular decomposition includes two reaction types: the cleavage of a methyl from the ring and ring-opening events.

During the initial consumption processes of MCP, five distinct alkylcyclopentane radicals are generated: CPTCH2 (primary radical), CYC5H9 (cyclopentyl radicals), MCPR2, MCPR3 (secondary radicals), and MCPR1 (tertiary radical).

The reaction flux study of the primary intermediates (radicals) produced from the initial decomposition of MCP has been conducted at 1300 K to un-

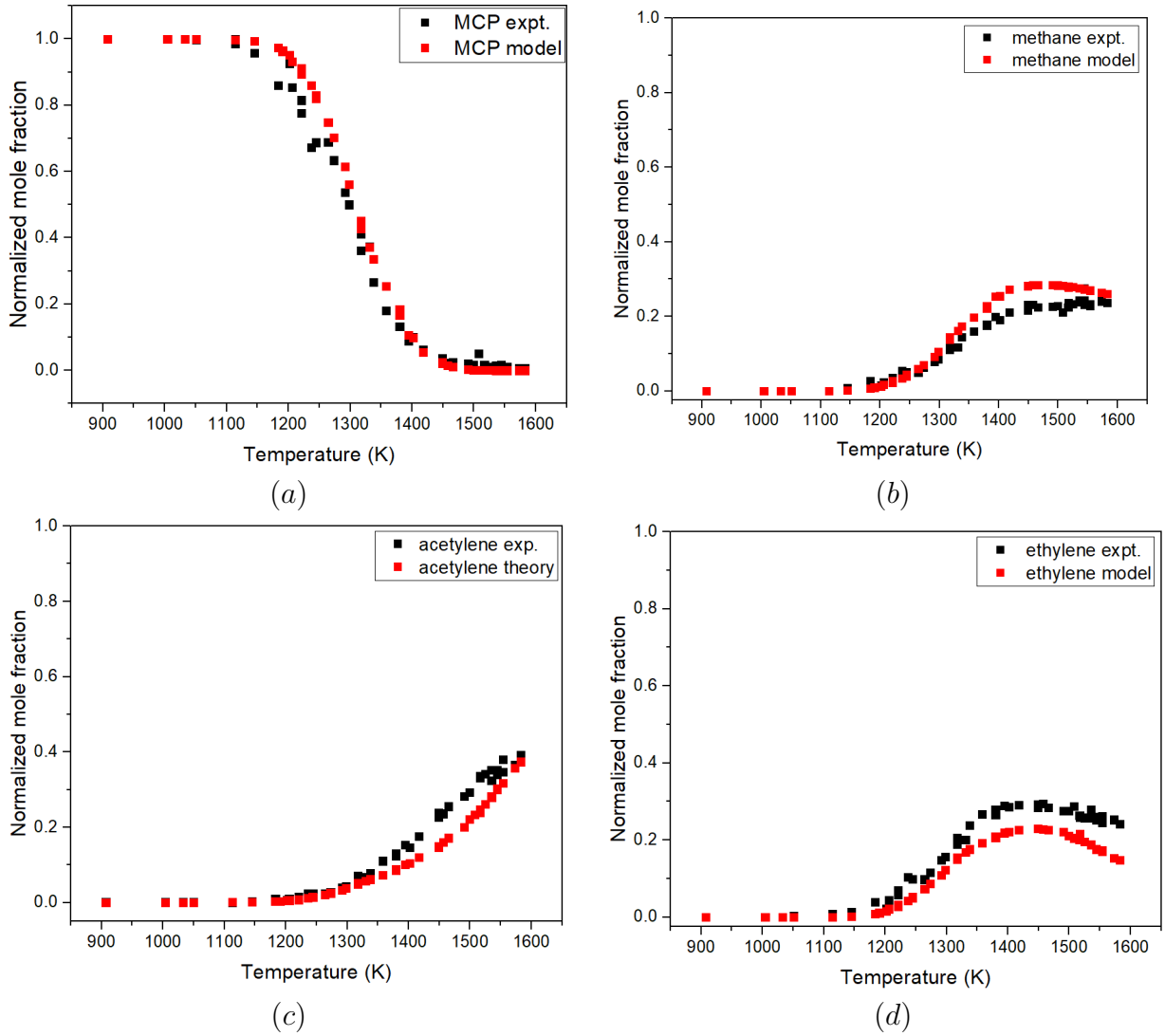


Figure 5.16: Experimental (symbols) and modeling (lines) results of major species of MCP pyrolysis. Normalization mole fraction for reactant $= [MCP]_t/k[MCP]_0$; Normalization mole fraction for products$[P_i]_t/k[MCP]_0$; where $k = [MCP]_t/[MCP]_0 + \sum_{i=1}^{15} \frac{[P_i]_t}{[MCP]_0}$

derstand the complex mechanisms of MCP pyrolysis. The reaction flux analysis of MCP at 1300 K, as predicted by the current model, is depicted in Fig. 5.17, showing a conversion of around 50%. The H-abstraction reaction significantly contributes to the consumption of alkylated cyclopentane and cyclohexane (methyl, ethyl, and isopropyl groups). The H-abstraction reaction plays a significant role in this case, with the primary pathway leading to the formation of the secondary radical and tertiary MCP radicals. In unimolecular dissociation reactions, the alkyl CH_3 elimination reaction is recognized as the primary C-C bond dissociation pathway. The figure indicates that MCP undergoes decomposition and isomerization, primarily yielding cyclopentyl and methyl radicals, as well as MCPR3, MCPR2, MCPR1, and CPTCH2, as the principal products via abstraction. The biradical formation pathways (INT1, INT2, and INT3) from MCP contribute minimally to its decomposition. The ring-opening isomerization process has a minimal impact on MCP consumption, accounting for only 3% of the total. A sensitivity study of MCP has been performed at 1300 K to better understand the influence of unimolecular decomposition and H-atom abstraction processes on MCP consumption (refer to Fig. 5.18 for the sensitivity analysis). The sensitivity analysis reveals that the most sensitive reaction is the dissociation of MCP into methyl and cyclopentyl radicals (CYC5H9) and H-abstraction reactions yielding MCP radicals (MCPR1, MCPR3, MCPR2, and CPTCH2). The positive impact of these reactions on MCP consumption came from their function as the primary consumption routes for MCP. As a result, hydrogen atom abstraction processes of MCP occur swiftly with the addition of extra hydrogen atoms or methyl radicals to the system. The negative effect comes from the consumption of the H and CH_3 radicals by other reaction pathways.

The decomposition and hydrogen abstraction of MCP produce cyclopentyl

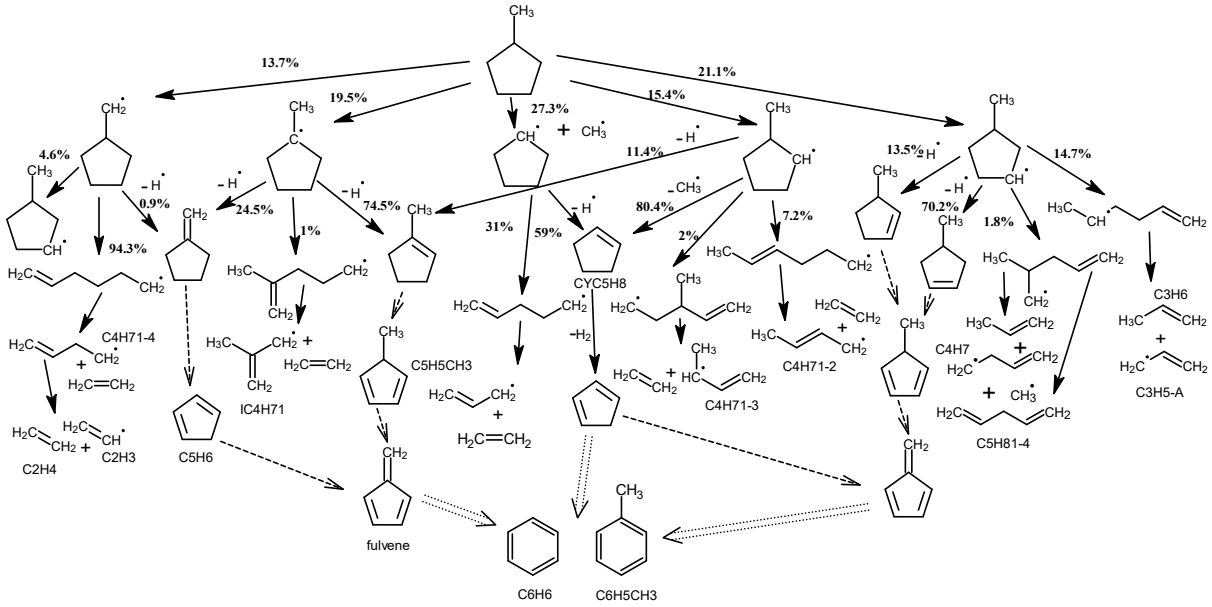


Figure 5.17: Reaction pathway analysis of the pyrolysis of MCP with different product formation at 1300 K. The solid lines shown are direct products, and the dashed lines shown are products formed from the shown products and other intermediates present in the reaction.

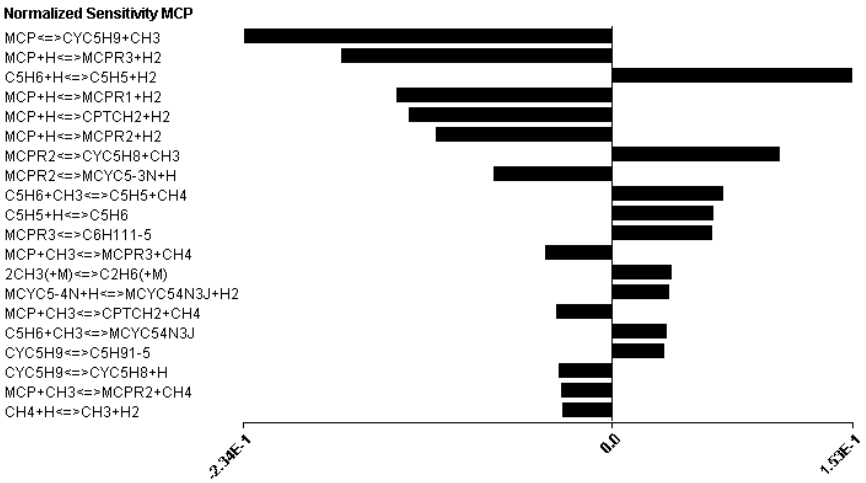


Figure 5.18: Normalized sensitivity analysis of MCP at a temperature of 1300 K with an approximate conversion rate of 50%.

and methylcyclopentyl radicals. The ring opening and subsequent decomposition of these radicals produce various components identified in this study. The subsequent discussion is structured according to the products identified from GC analysis of the thermal decomposition.

5.5.2 Formation of C5–C1 species

This study examined various C5–C1 species, including alkanes, alkenes, and alkynes, specifically methane, ethene, and acetylene. The product concentration profiles indicate that methane (CH_4), acetylene (C_2H_2), and ethylene (C_2H_4) are the predominant products resulting from the decomposition of MCP. Following ethylene, concentrations of methane and acetylene are also shown to be high. C3 compounds, including allene (aC_3H_4), propene (C_3H_6), and propyne (pC_3H_4), exhibit similar trends. The compounds start formation at approximately 1200 K, peak around 1350 K, and thereafter decrease.

1,3-butadiene (C_4H_6), vinylacetylene (C_4H_4), and but-1-ene (C_4H_8) are C4 compounds produced during the decomposition of MCP, but in lesser quantities. Cyclopentene (C_5H_8) and cyclopentadiene (C_5H_6) are important cyclic C5 compounds that begin formation at the same temperature as aromatic benzene formation (1250 K), peaking about 1400 K before subsequently decreasing with temperature.

As shown in Fig. 5.17, the ring-opening isomerization of cyclopentyl and alkylcyclopentyl radicals produces an alkenyl radical, methyl cyclopentene, and cyclopentene. They produce a variety of compounds, such as hexene (hex-2,1-enes) and methylpentene (2,3,4-methylpentenes), along with radicals. These linear chain compounds further undergo beta-scission reactions to yield an abundance of smaller constituents, including 1,3-butadiene, ethene, propene,

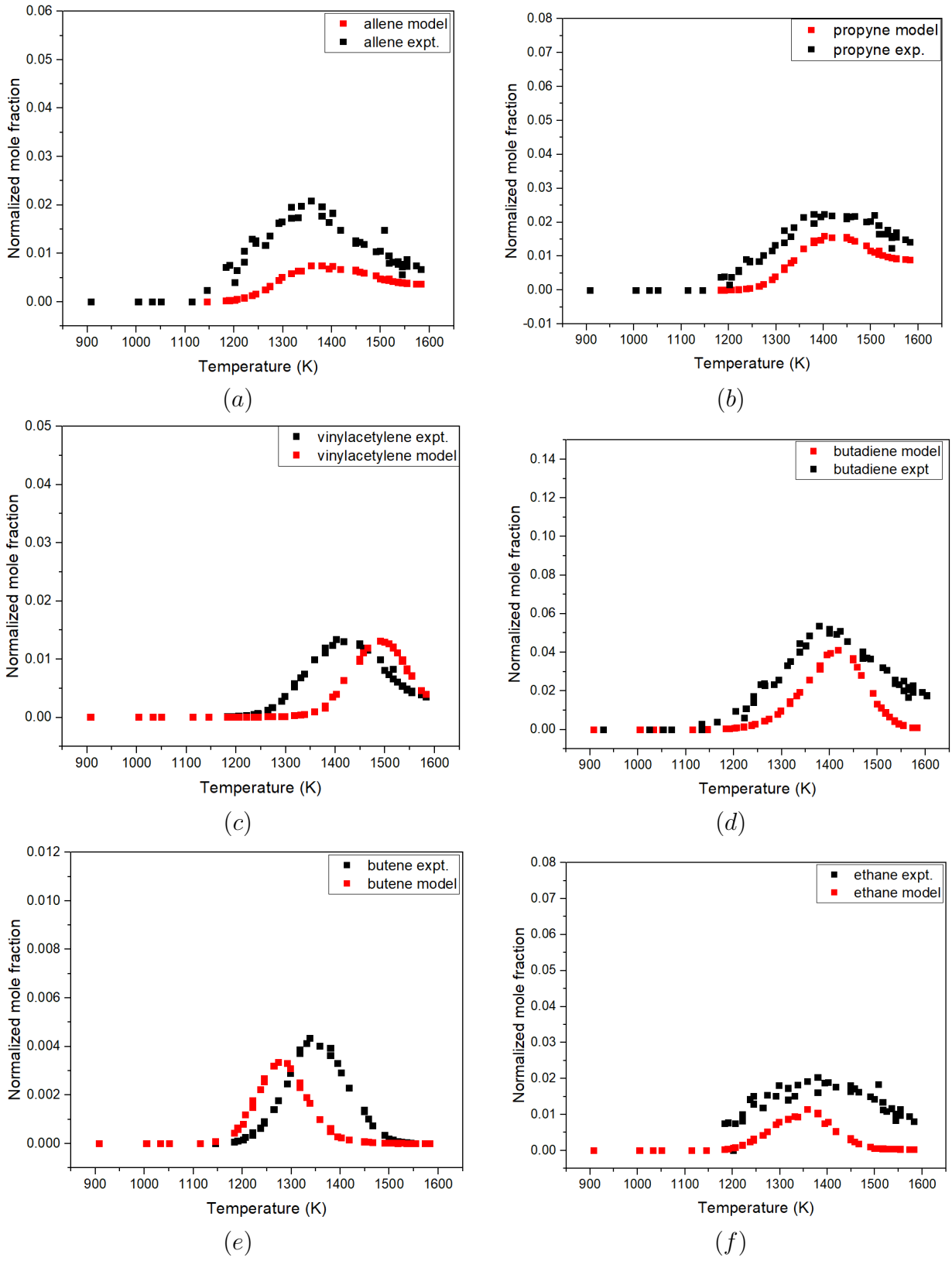


Figure 5.19: Experimental (symbols) and modeling (lines) results of major species of MCP pyrolysis. Normalization mole fraction for reactant $= [MCP]_t/k[MCP]_0$; Normalization mole fraction for products$=[P_i]_t/k[MCP]_0$; where $k = [MCP]_t/[MCP]_0 + \sum_{i=1}^{15} \frac{[P_i]_t}{[MCP]_0}$

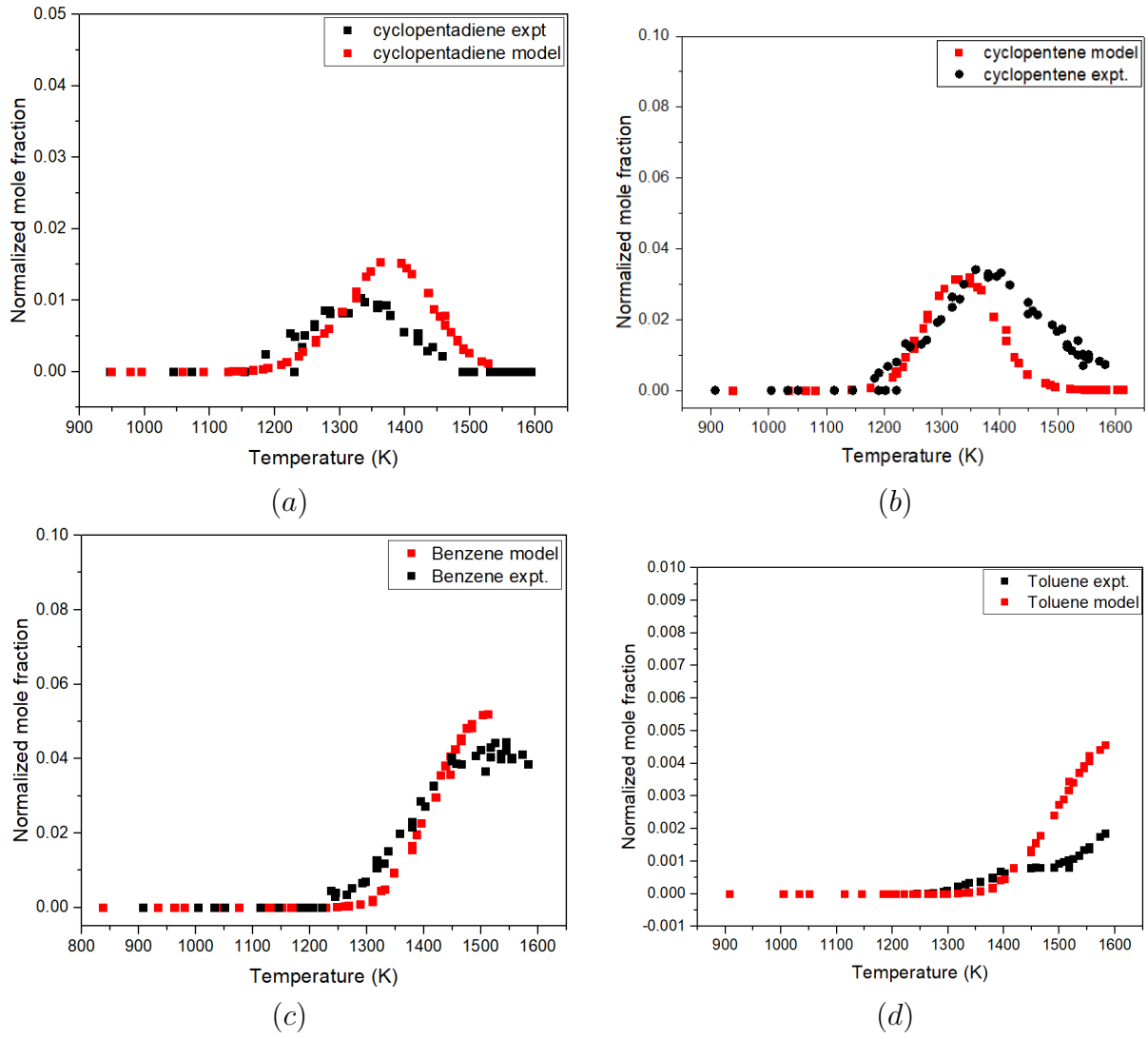


Figure 5.20: Experimental (symbols) and modeling (lines) results of major species of MCP pyrolysis. Normalization mole fraction for reactant $= [MCP]_t/k[MCP]_0$; Normalization mole fraction for products$=[P_i]_t/k[MCP]_0$; where $k = [MCP]_t/[MCP]_0 + \sum_{i=1}^{15} \frac{[P_i]_t}{[MCP]_0}$

and butene, as well as radicals such as CH_3, C_2H_5, C_3H_7, C_4H_9, etc. These steps encompass the synthesis of all C1-C5 products and the aromatic compounds generated during pyrolysis.

5.5.3 Formation of benzene and toluene

Benzene and toluene are the aromatic products found in the MCP pyrolysis. Aromatics like benzene and toluene are predominantly generated through the addition of resonance-stabilized radicals. Resonance-stabilized radicals like al-

lyl, propargyl, butadiene, phenyl radical, and benzyl radical are thought to be crucial in the pyrolysis conditions that lead to the synthesis of aromatics. These radicals have longer lives than ordinary radicals, which allows them to build up to comparatively high concentrations. Recombination events with other radicals or intermediates result in an increase in molecular weight and are significant consumption pathways for these resonance-stabilized radicals. For MCP, benzene is produced via the self-recombination process of propargyl radicals (C_3H_3+C_3H_3), the combination of propargyl radicals with allene and propyne (C_3H_3+C_3H_4-A, C_3H_3+C_3H_4-P), the combination of benzyl and allyl radicals (C_5H_6+C_2H_3), combination of butadiene radicals with allyl radicals and acetylene (C_4H_5-N+C_2H_3, C_4H_5-N+C_2H_2). Fulvene is the most important intermediate in the production of benzene (for example, FULVENE+H=C_6H_6+H and FULVENE=C_6H_6). The benzyl radical eventually reacts with H, C_2H_3, and C_5H_6 to give benzene. Fulvene significantly contributes to benzene formation, accounting for 30% of the total production. Fulvene is formed by various processes, such as the addition of propargyl radicals (C_3H_3+ C_3H_3), as well as through reactions between propargyl and allyl radicals (C_3H_3+C_3H_5-A) and between acetylene and 1,3-butadiene radicals (C_4H_5-N + C_2H_2) and (C_4H_5-I + C_2H_2).

Toluene is a minor product formed during the MCP pyrolysis process. The main source of toluene (almost 85%) is the combination of an H-atom/H_2 with a benzyl radical ($C_6H_5CH_2$), which is generated via the addition of acetylene to the cyclopentadienyl radical (C_5H_5 + C_2H_2). The toluene is also formed from benzene (almost 5%) via C_6H_6+CH_3 and $C_6H_5CH_2$+C_6H_6 reactions. Other relevant reactions between smaller intermediates include the reaction between a propargyl radical and 1,3-butadiene (C_3H_3+C_4H_6), as well as the reaction between butadiene radicals and allene and propene. (C_4H_5-N+C_3H_4-A, C_4H_5-

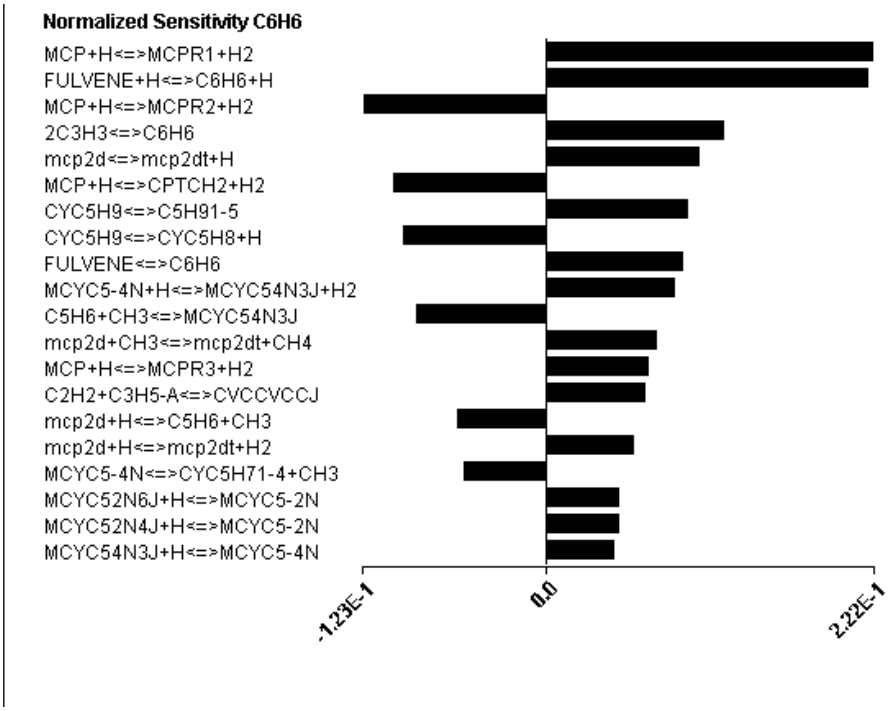


Figure 5.21: Normalized sensitivity analysis of benzene during MCP pyrolysis at 1400 K, with an MCP conversion rate of approximately 85 %

N+C_3H_4-P).

5.5.4 The rate constant of the overall decomposition of MCP

The overall rate coefficient for the thermal decomposition of MCP has been determined throughout the temperature range of 1050 K to 1526 K using the following equation.

$$k = -\frac{1}{t} ln \frac{MCP_t}{MCP_0}$$

In this context, t represents the reaction time (dwell time), MCP_0 denotes the initial concentration of MCP, and MCP_t indicates the concentration of IPCH after time t. The rate constant expression is derived from the linear fitting of the data presented in Fig. 5.22.

$$k(s^{-1}) = 10^{11.3 \pm 0.3} exp \frac{(-39.1 \pm 1.7) kcal/mol}{RT}$$

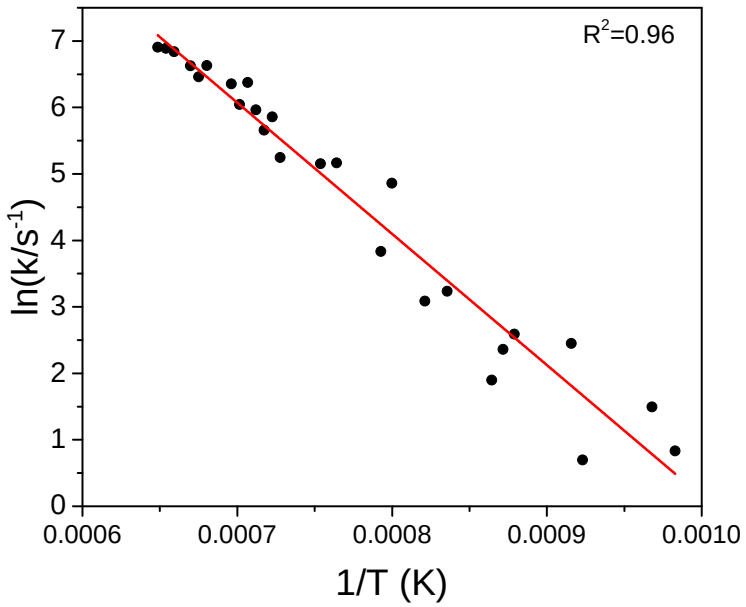


Figure 5.22: Arrhenius plot of overall decomposition of MCP

5.6 Conclusion

This study investigates the thermal decomposition of MCP using both experimental and computational techniques. This study serves as the basis for investigating the kinetics of MCP and alkylated cyclopentane pyrolysis, which are constituents of aviation fuels and gasoline.

1. The initial steps include unimolecular decomposition (loss of-H and -methyl groups) and ring-opening isomerization of MCP. MCP exhibits three open-ring isomerization pathways through the cleavage of the C-C bond at three different positions, resulting in biradicals. The potential energy surfaces for the ring-opening isomerization pathways and the methyl loss reaction of MCP have been calculated in detail using the multireference method (MRCI//CASSCF). The methyl group dissociation barrier in MCP is lower than that for the C-C bond in the ring of MCP, similar to MCH. The ring-opening isomerization of MCP reveals that the

dissociation of the C–C bond adjacent to the methyl group has a lower energy barrier compared to the other C–C bond dissociation within the ring. These observations coincide with similar trends noted in the calculations of IPCH, MCH, and ECP. Comparisons between cycloalkanes and alkylated cycloalkanes indicate that reactivity increases with the addition of side-chain alkyl groups.

2. Based on quantum chemical calculations, the temperature-dependent (800-2000 K) high-pressure limit rate constants of the unimolecular reactions were calculated. Our calculations indicate that the competition between dissociation (loss of the methyl group) and ring-opening isomerization pathways exhibits a strong temperature dependence. Unimolecular decomposition of MCP is dominant over the isomerization reactions. The HPL thermal rate constants for all elementary reactions of MCP radicals in the modified Arrhenius expression have been established for the temperature range of 800-2000 K, pertinent to kinetic modeling studies of MCP pyrolysis and oxidation. Finally, a kinetic model for MCP has been established based on the preceding computations, comprising 426 species and 1354 reactions.

3. The pyrolysis of MCP was experimentally examined by analyzing species distribution within the shock tube at temperatures ranging from 950 to 1600 K and pressures between 10 and 25 bar. The kinetic model offers qualitative predictions that correlate well with experimental data. Based on the experimental and simulation research, we could conclude that:

    - The predominantly produced compounds are methane, acetylene, ethylene, propene, 1,3-butadiene, 1-butene, and cyclopentadiene.
    - Benzene and toluene are the aromatic compounds found in the ex-

periment.

- ROP and sensitivity analysis result in the following conclusions: The unimolecular decomposition of MCP initiates with methyl dissociation and abstraction processes that primarily consume MCP. Furthermore, the MCP radical dissociation leads to the formation of various smaller and larger hydrocarbon products. Resonance-stabilized radicals, including allyl, propargyl, butadienyl, phenyl, and benzyl radicals, are essential in the pyrolysis conditions that promote the synthesis of aromatics like benzene and toluene during MCP pyrolysis.

The overall decomposition rate of HYD/MCP has been determined and is expressed as follows.

$$k(s^{-1}) = 10^{11.3\pm0.3} exp \frac{(-39.1 \pm 1.7) kcal/mol}{RT}$$

This study's experimental and kinetic analyses aim to improve understanding of unimolecular decomposition pathways and the reaction mechanisms relevant to the synthesis of smaller alkanes, alkenes, and cycloalkanes, particularly aromatic compounds derived from monoalkylated cyclopentane and related alkylated cyclopentanes. The findings suggest that MCP, being the most basic monoalkylated cyclopentane, can serve as an efficient surrogate for alkylcycloalkanes found in gasoline and naphtha fuels.

Chapter 6

Conclusion and future perspectives

This thesis presented the details of shock tube investigations focused on astrochemistry and combustion, performed in two separate experimental setups. The sections that follow examine the significant contributions made in each facility and the key conclusions made. Possible future directions for shock-induced studies are also put forward.

6.1 Astrochemistry studies in the MST facility

6.1.1 Important contributions

The primary contributions to the experimental facilities include the development of the Material Shock Tube (MST) facility, the addition of multiple optical measurement systems, and the development of a time-resolved broadband emission spectrometer.

Important experimental investigations include the thermal decomposition analysis of PAHs, fullerenes, and hydrocarbons. The comparison of C_2 emission from PAHs, hydrocarbons, and fullerenes using real-time in situ measurements

was the major focus of our study. This real-time analysis was supplemented by ex-situ measurements of the shocked final products.

6.1.2 Important findings

The laboratory shock processing of cosmic dust analogs, particularly polycyclic aromatic hydrocarbons (PAHs) and fullerenes, was investigated in the MST facility to gain a deeper understanding of the physical and chemical changes that occur during shock processing. Major outcomes from the shock tube study of PAH, fullerene, and hydrocarbons can be classified into two categories: in situ and ex situ results. In the context of in situ real-time spectroscopy, the spectra of C_2, small C_nH_x clusters (broad green component), and black body emission were found. In the ex situ studies, the most important outcome was the observation of graphenic/graphitic nanostructures (carbon nano-onions, nanotubes, and nanoribbons) in the post-shock samples.

Finally, we conclude that the shock waves drive the transformation of PAHs into small hydrocarbons and carbon clusters, which recombine in the cooling phase into graphene-like structures, affecting the carbon lifecycle of the interstellar medium. The identification of C_nH_x species as potential carriers of a broad green emission seen in the laboratory suggests a possible link to the λ5450 diffuse interstellar band. This research underscores the importance of shock tubes in simulating astrophysical conditions and investigating the chemical evolution of large molecules and small particles in space. The findings and the new research facility will enhance the astrochemistry/astrophysics community's understanding of dust evolution and the carbon lifecycle in the interstellar medium.

6.1.3 Future perspectives

The integration of diverse expertise, including experiments, chemical analysis, theoretical approaches, and observations, is supported by the presence of unique shock tube facilities. The long-term objectives include enhancing the understanding of the carbon life cycle in the ISM, identifying new shock tracers within the ISM, and understanding the relationship between hydrocarbons, aromatics, PAHs, fullerenes, and soot formation in the ISM.

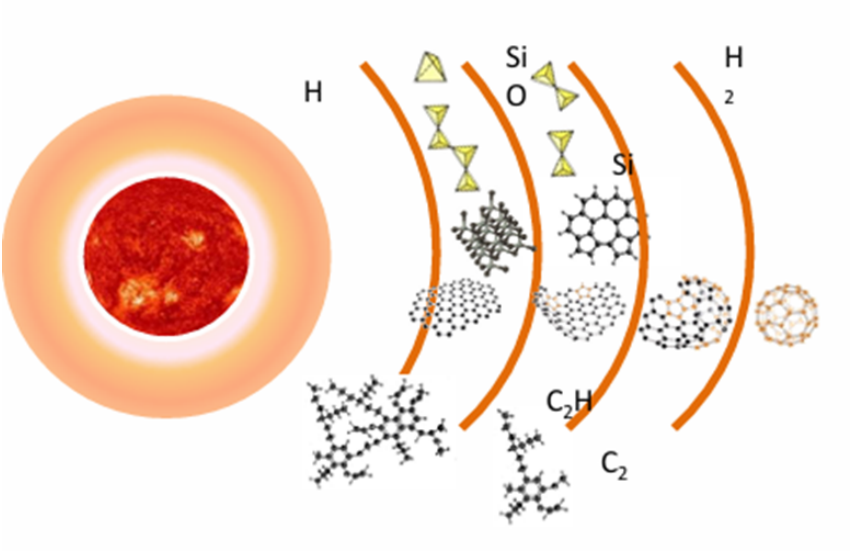


Figure 6.1: Focus on understanding the carbon lifecycle in ISM

Figure 6.1 illustrates the conceptual framework of dust and molecular formation within the circumstellar envelope of a carbon-rich star, such as an AGB star. This illustrates the progression of simple atoms and molecules from the hot stellar photosphere to larger carbonaceous clusters, ultimately resulting in soot-like nanoparticles or fullerenes. Future plans involve examining various interstellar carbon dust analogs, including silicates, SiC (silicon carbide), PAHs, and graphene, in the context of interstellar shock propagation to understand such phenomena. Certain objectives may be attained through the study of shock tubes. Finally, the incorporation of time-of-flight mass measurements via a shock tube can also facilitate the investigation of transient species during

shock processing, leading to more profound conclusions.

6.2 Combustion studies in the CST facility

6.2.1 Important contributions

The main contributions to the experimental facilities consist of the automation of the CST facility, the addition of various optical measurement systems, and the temperature calibration of the CST facility. Important studies involve the development of a comprehensive kinetic model for the pyrolysis of hydrindane and methylcyclopentane, based on both experimental data and theoretical calculations.

6.2.2 Important findings

The primary results from the shock tube investigation of hydrocarbons can be categorized into two distinct groups: theoretical and experimental. The key theoretical finding indicates that the first step in the thermal decomposition of hydrindane and methylcyclopentane involves ring-opening C-C dissociation and C-CH_3 bond dissociation, rather than C-H bond dissociation. Figure 6.2 illustrates frequently observed monocyclic, bicyclic, and branched cyclic molecules in fuel, and the theoretical analysis has been performed for a comparative analysis of the reactivity of surrogate molecules.

Comparison of the surrogate molecule reactivity

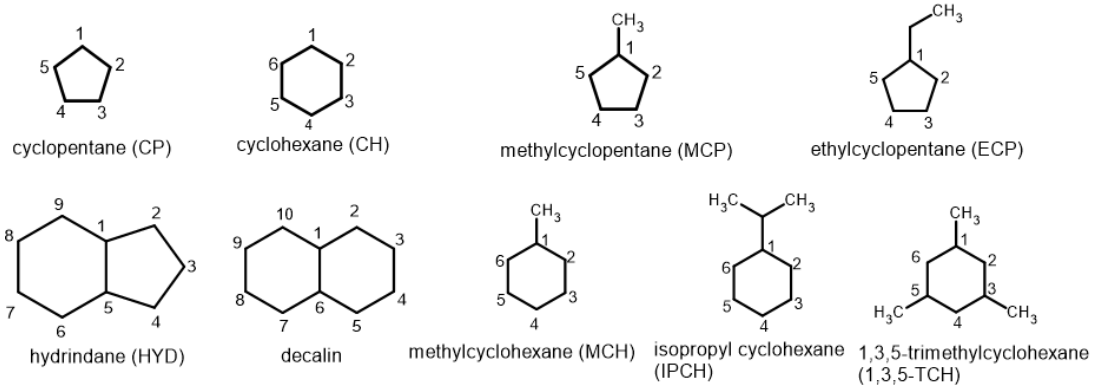


Figure 6.2: Monocyclic, bicyclic, and branched cyclic molecules in fuel

Table 6.1 below illustrates the comparison of reactivity among monocyclic, bicyclic, and branched cyclic compounds. From the comparison, we can conclude that the reactivity of cycloalkanes increases owing to the side chain branching, as it possesses the lowest C-C bond dissociation energy. The reactivity among cyclopentane and cyclohexane derivatives is as follows: ECP $>$ MCP $>$ CPT and IPCH$>$MCH$>$135-TCH$>$CH. In bicyclic molecules such as hydrindane and decalin, the reactivity is similar, and the dissociation of the C-C bond initiates the unimolecular decomposition process. This thesis covered two important categories of molecules: the MCP and HYD.

Table 6.1: Comparison between the reactivity of monocyclic, bicyclic, and branched cyclic molecules. where CPT=cyclopentane, MCP=methyl cyclopentane, ECP=ethyl cyclopentane, CH=cyclohexane, MCH=methyl cyclohexane, IPCH=isopropyl cyclohexane, and 135-TCH=1,3,5-trimethylcyclohexane, HYD=hydrindane. Energy: kcal/mol

	CPT[a]	MCP[b]	ECP[c]	CH[d]	MCH[e]	IPCH[f]	135-TCH[g]	HYD[h]	decalin[i]
Unimolecular decomposition									
C-H dissociation	97.5	101.5,95.9,97.7,97.4	-	97.8	-	-	-	95.4,98.9,97.5,99.1,100.5	97.0,102.4,99.9
CH_3 elimination	-	84.7	84.5	-	84.0	83.2	85.6	-	-
C_2H_5 elimination	-	-	79.3	-	-	-	-	-	-
C_3H_7 elimination	-	-	-	-	-	81.6	-	-	-
Ring-opening isomerization									
TS of C1-C2	85.9	86.3	86.2	88.7	-	85.9	86.3	82.3	85.4
TS of C2-C3	-	86.5	85.7	-	85.0	88.0	-	83.6	84.0
TS of C3-C4	-	86.0	86.8	-	89.0	87.6	-	-	86.9
TS of C5-C6	-	-	-	-	89.0			86.7	-
TS of C6-C7	-	-	-	-	-			91.6	-
TS of C7-C8	-	-		-	-			89.4	-

[d]CASPT2/cc-pVDZ [259] [e]CASPT2/cc-pVDZ [261] [f,g,i]MRCI [130]. [a,b,c,h]MRCI (This work).

Finally, the experimental studies of MCP and HYD in the CST facility result in the formation of small hydrocarbons, cycloalkanes, and aromatic compounds, which are confirmed through complementary mechanistic studies, thereby improving the understanding of aromatic formation in pyrolysis investigations. The kinetic modeling indicates that the resonance-stabilized radicals, such as allyl, propargyl, butadienyl, phenyl, and benzyl radicals, play a crucial role in

pyrolysis conditions that facilitate the synthesis of aromatics, including benzene and toluene. We can also conclude that the complexity of the molecular structure and the increase in carbon and hydrogen numbers correlate with an increase in the number of products and possible reactions; for example, HYD exhibits a greater variety of products compared to MCP.

6.2.3 Future perspectives

The availability of specialized shock tube facilities facilitates the integration of diverse expertise, including both experimental and theoretical approaches. The primary objectives are to investigate combustion processes in various engines and to explore the correlation between hydrocarbons, aromatics, and soot formation using these methods, as well as to develop accurate kinetic models for such processes.

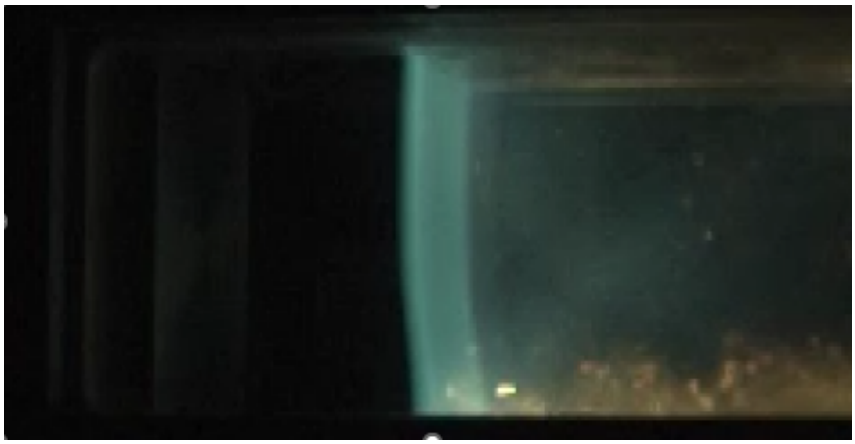


Figure 6.3: Flame visualization in the CST facility

Future plans involve the potential integration of a multispecies broadband spectral monitoring system utilizing cavity-based absorption or emission spectroscopy, alongside high-speed visualization techniques. The visualization of flame and ignition in shock tubes is depicted in Figure 6.3, illustrating a study that captures flame propagation following autoignition within the CST facility.

This was carried out using the Phantom v310 high-speed camera operating at a rate of 100,000 frames per second. This experiment was conducted after completing the thesis work. It is hoped that this facility will be used to gain a fundamental understanding of flame initiation and propagation in the shock tube facilities in our laboratory.

Appendices

Appendix A

Reaction mechanisms

A.1 Reaction mechanism of hydrindane

ELEMENTS H C AR END

SPECIES

!=====C0 AR H H2

!=====C1 C CH CH2 CH2* CH3 CH4

!=====C2 C2H C2H2 H2CC C2H3 C2H4 C2H5 C2H6

!=====C3 C3H2 C3H3 aC3H4 pC3H4 aC3H5 CH3CCH2 CH3CHCH C3H6 nC3H7 iC3H7 C3H8

!=====C4 C4H C4H2 nC4H3 iC4H3 C4H4 nC4H5 iC4H5 C4H5-2 c-C4H5 C4H6 C4H612 C4H6-2 SAXC4H7 C4H7 iC4H7 iC4H7-1 C4H7-2 CH3CCHCH3 C4H8-1 C4H8-2 iC4H8 pC4H9 sC4H9 tC4H9 iC4H9

!=====C5

P1XCH2C4H5-13E S4XC4H4-13E2M S1XC4H4-13E2M T1XC5H7-14E T4XC5H7-13E T1XC5H7-13E C5H8-14E C5H8-13E C5H8-12E C4H5-13E2M S3XC5H9-1E P5XC5H9-1E S4XC5H9-1E S4XC5H9-2E P5XC5H9-2E P4XC4H6-1E2M P4XC4H6-1E3M C5H10-1E C5H10-2E P1XC5H11 S2XC5H11 S3XC5H11 ! cC5H7 to cC5H71-3

PAXCH2-2-1C4H7 P1XC4H82M cC5H10 cC5H9 cC5H8 cC5H71-4 cC5H71-2 cC5H71-3 P5XC5H7-13E P5XC5H7-14E CH2cC5H8 CH2S2XcC5H7

C4H7-1E3M C4H7-2E2M P4XC4H6-2E2M P4XC4H83M S2XC4H83M T2XC4H6-1E3M S1XC4H6-1E3M

!=====C6

S1XcC6H7-24E C6H8-135E cC6H8-13E S2XcC6H9-1E S3XC6H9-15E P6XC6H9-13E S5XC6H9-13E cC6H10 cC6H9 C6H10-13E C6H10-15E cC6H11 P1XCH2cC5H9 S3XcC5H81M P6XC6H11-1E S5XC6H11-1E S4XC6H11-1E S3XC6H11-1E P5XC5H8-1E4M C6H12-1E cC6H12 S3XcC6H9-1E cC6H8-14E

C2H3-2-PXC4H6 C2H3-3-PXC4H6 C6H10-14E P6XC6H11-2E P6XC6H11-3E PXC2H4-2-1C4H7 PXCH2-3-1C5H9 S4XC6H11-2E CH3S2XcC5H8 P5XC5H8-1E3M CH2-3-C6H8-14 S3XC5H102M S3XC5H8-1E4M P5XC5H8-2E2M P3XC3H4-1E2IP P1XCH2C4H6-1E3M P1XC5H104M P1XC5H8-2E4M P1XC4H723M C6H12-2E C5H9-2E2M C5H7-13E4M C5H9-1E4M C5H9-2E4M

cC5H74M cC5H75M S3XcC5H64M S3XcC5H65M C4H6-1E23M

!=====C7

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S4XC7H11-15E S7XC7H11-15E T3XC6H8-15E3M S3XC6H8-15E2M S4XC6H8-15E3M P1XCH2-3C6H9-15E S4XC6H8-15E2M P1XCH2C6H9-15E C7H12-13E C7H12-16E C7H12-15E C7H12-24E C6H9-15E3M CH2-3-C6H10-1E C6H9-15E2M C6H9-13E5M CH2cC6H10 MCH-1E MCH-2E MCH-3E PXCH2cC6H11 T1XMCH S2XMCH S3XMCH S4XMCH P6XC6H10-1E2M P7XC7H13-2E P6XC6H10-1E3M S6XC7H13-1E P7XC7H13-1E S3XC7H13-1E P6XC6H10-1E4M P6XC6H10-1E5M S3XC6H10-1E5M S4XC7H13-2E S3XC6H10-1E4M S3XC6H10-1E2M T3XC6H10-1E3M MCH C7H14-1E C7H14-2E C6H11-1E2M C6H11-1E3M C6H11-1E4M C6H11-1E5M

C2H3TXcC5H8 C2H3S2XcC5H8 C2H3S3XcC5H8 P7XC7H11-13E S3XC7H11-16E CH2S3XcC6H9 CH2S4XcC6H9 CH2-4-PXC6H9 CH2-5-PXC6H9 C2H3-2-PXC5H8 C2H3cC5H9 PAXCH2-2-1C6H11

C4H5-13E2IP C4H7-1E2IP C5H8-1E34M C6H9-14E5M C6H11-3E2M P4XC4H6-1E2IP P4XC4H6-1E3IP P6XC6H10-2E2M S4XC6H10-1E5M P1XC6H10-3E5M

! ECH Species

!=====C8

!C8H9 CH2CH-1-SAXcC6H6 CH2CH-2-SAXcC6H6 CH2CH-3-SAXcC6H6 CH2CH-4-SAXcC6H6 CH2CH-5-SAXcC6H6 !C8H10 CH2CH-1-cC6H7-13 CH2CH-2-cC6H7-13 !C8H11 CH2CH-2-SAXcC6H8 CH2CH-1-SAXcC6H8 C2H5-1-SAXcC6H6 C2H5-4-SAXcC6H6 CH3CH-1-cC6H7-13 C2H5-3-SAXcC6H6 C2H5-2-SAXcC6H6 CH3CH-2-cC6H7-13 C2H5-6-SAXcC6H6 C2H5-5-SAXcC6H6 !C8H12 C2H5-1-cC6H7-13 C2H5-2-cC6H7-13 C2H5-5-cC6H7-13 !C8H13 CH2CH-1-cC6H10 C2H5-1-SAXcC6H8 C2H5-2-SAXcC6H8 CH3CH-1-cC6H9 C2H5-4-SAXcC6H8 C2H5-3-SAXcC6H8 C2H5-5-SAXcC6H8 C2H5-6-SAXcC6H8 C2H3-2-PXC6H10 CH2CH-2-cC6H10 CH2CH-3-cC6H10 CH2CH-4-cC6H10 PXC8H13-13 C2H3-3-PXC6H10 SAXC8H13-17 C2H3-4-PXC6H10 C2H3-5-PXC6H10 !C8H14 CH2CHcC6H11 CH3CHcC6H10 C2H5-1-cC6H9 C2H5-3-cC6H9 C2H5-4-cC6H9 C8H14-13E C2H3-2-1C6H11 CH3CH-2-1C6H11

!C8H15 P8XC8H15-2E C2H5-2-PXC6H10 C2H5-3-PXC6H10 P8XC8H15-3E PXC2H4-4-1C6H11 S6XC8H15-1E PXCH2-5-1C7H13 S4XC8H15-2E C2H5-2-SAX1C6H10 C2H5-3-TAX1C6H10 S5XC8H15-3E C2H5-4-SAX1C6H10 S3XC7H12-1E5M P8XC8H15-1E S3XC8H15-1E SXC2H4cC6H11 PXC2H4cC6H11 C2H5TXcC6H10 C2H5S2XcC6H10 C2H5S3XcC6H10 C2H5S4XcC6H10 C3H7-3-SXC5H8 C2H5-3-SXC6H10 C2H5-4-SXC6H10 P7XC7H12-1E3M T3XC7H12-1E3M P8XC8H15-4E C2H5-3-S2XC6H10 P1XCH2C6H9-15E P1XCH2-4C6H915E

!C8H16 C8H16-1E C8H16-2E C8H16-3E C7H13-1E5M C2H5cC6H11

S1XcC5H65IP C8H14-16E C7H11-15E6M C7H11-15E5M C7H11-14E6M C5H7-14E3IP C5H7-14E2IP C5H7-13E3C3H7 C8H14-17E

! aromatic species

!=====C5 C5H3 cC5H4 C5H4 lC5H5 C5H5 C5H6 lC5H7 C5H52 C5H2

!=====C6 A1 A1- l-C6H4 o-C6H4 n-C6H5 fulvene C6H2 C6H3

!=====C7 A1CH3 A1CH2 C7H6 C7H5 C5H5CH2-2 C5H5CH2-3 C5H5CH2-1 C6H4CH3 A1CH

cC5H5-13E1M cC5H5-13E5M

!=====C8 A1CC A1C2H- C6H3C2H A1C2H A1cC2H2 A1CCH2 A1CHCH C6H4C2H3 A1C2H5 A1CH2CH2 A1CHCH3 A1C2H3 C6H4C2H5

!=====C9 C9H7 C9H8 C9H9-1 C9H10

TXIPCH T5XC6H10-1E5IP T4XC6H10-1E4IP T3XcC5H8CH2IP T3XC6H10-1E3IP T1XIPCH P8XC8H14-2E2M S7XC8H14-3E2M S7XC8H14-2E2M S7XC8H14-1E7M S6XC8H14-3E2M S6XC8H14-2E2M S6XC8H14-1E7M S5XC8H14-3E2M S5XC8H14-2E2M S5XC8H14-1E7M S5XC6H10-1E4IP

S5XC6H10-1E3IP S5XC6H10-1E2IP S4XIPCH S4XcC5H71M5IP S4XC8H14-2E2M S4XC8H14-1E7M S4XC6H10-1E5IP S4XC6H10-1E3IP S4XC6H10-1E2IP S3XIPCH S3XcC5H71M5IP S3XcC5H71M4IP S3XcC5H71M1IP S3XC8H14-1E7M S3XC6H10-1E5IP S3XC6H10-1E4IP S3XC6H10-1E2IP S2XIPCH S2XcC5H51M1IP S2XcC5H6-3ECH2IP S1XIPcC5H9 PXIPCH P8XC8H14-3E2M P8XC8H14-1E7M P6XC6H10-1E5IP P6XC6H10-1E4IP P6XC6H10-1E3IP P6XC6H10-1E2IP P1XCH2cC5H85IP P1XCH2cC5H84IP P1XCH2cC5H81IP IPCH-3E IPCH-2E IPCH-1E IPCH CH2-IPCH CH2-2-IPCH cC5H61M5IP cC5H61M1IP cC5H7-3ECH2IP C8H15-3E2M C8H15-2E2M C8H15-1E7M C6H11-1E5IP C6H11-1E4IP C6H11-1E3IP C6H11-1E2IP int1 int2 int3

!=====aromatic

S6XIPCH-1E IPCH-15E S4XIPCH-15E S3XIPCH-15E A1IP PXA1IP T1XIPCH-2E S2XIPCH-3E IPCH-13E S6XIPCH-13E S5XIPCH-13E

!=====decalin submechanism

decalin biradical1 biradical2 biradical3 C6H10-1E56CH P6XC6H9-1E12CH P4XC4H8cC6H9 TXC4H8cC6H9 P1XC9H15-3E5CH2 S1XC6H9-1E12CH S3XC6H9-1E56CH T1Xdecalin S2Xdecalin S3Xdecalin decalin-1bE decalin-1E decalin-2E decalin-3E C6H10-1E45CH C6H10-1E34CH P6XC6H9-1E23CH P6XC6H9-1E34CH P6XC6H9-1E45CH S1XC4H8cC6H9 T3XC6H9-1E23CH S1Xspiro-4-5-DN P1XCH2-1-HD P1XCH2-2-HD P1XCH2-3-HD S8XHD-1M HD-7E1M S6XHD-7E1M HD-57E1M S4XHD-57E1M HD-357E1M S2XHD-357E1M indene S4XHD2M HD-4E2M T1XHD-4E2M HD-14E S6XHD-14E HD-146E S8XHD-146E P1XCH2-3-HD T1XHD3M HD-1bE3M S2XHD-1bE3M HD-1b2E S6XHD-1b2E HD-1b26E S7XHD-1b26E decalin-1bE S2Xdecalin-1bE decalin-1b2E S4Xdecalin-1b2E tetralin S7Xdecalin-1b24E S9Xdecalin1b247E naphthalene decalin-1b2E T1Xdecalin-2E T6Xdecalin-1E S3Xdecalin-15E S2Xdecalin-3E decalin-13E T6Xdecalin-13E C2H3cC5H9 C2H3T1XcC5H8 C2H3cC5H7 C2H3S3XcC5H6 C2H3cC5H5 C2H3C2H3cC5H8 C5H9-1EcC5H7 C5H9-1EcC5H6 C5H9-1EcC5H5 S6XcC10H17-1E P1XC10H17-46E S1XC10H17-16E P1XC8H13-45-CH2 S4XcC10H17-1E S1XC10H17-19E P10XC10H17-16E S3XcC10H17-1E P10XC10H17-14E P10XC10H17-17E S6XC10H17-13E S3XC10H17-19E S5XC10H17-19E S5XC10H17-16E S5XC10H17-13E S4XC10H17-19E S4XC10H17-16E S6XC10H17-17E S7XC10H17-15E S1XC3H4CH3cC6H10 C3H5P1XCH2cC6H10 C4H7S2XcC6H10 S3XC6H9-1E45CH P1XC5H8-1EcC5H9 C5H9-1ES2XcC5H8 S1XC3H6C2H3cC5H8 S1XC4H8cC6H9-2E C5H9-1EcC5H8 C2H3cC6H9 C2H3T1XcC6H10 C2H3T1XcC6H8-2E C2H3cC6H11 C2H3cC6H9-2E C3H5CH3S3XcC6H9 C3H5CH3cC6H8-2E DCH-15E o-xylene CH2-12-cC6H8 S3XDCH-15E T3XC6H9-1E34CH P9XC9H14-13E5M P8XC8H14-1E4C2H3 P10XC10H17-15E S9XC10H17-13E S4XC10H17-19E

S6XC6H9-1E56CH PXC2H4cC6H9-2E TXC4H9cC6H8 nC4H9cC6H7 PXC2H4cC6H9-1E PXCH2CH2cC6H9 P8XC8H14-3E4C2H3 P7XC7H10CH2C2H5 P8XC8H14-1E5C2H3 P10XC10H17-13E C7H10-136E

P1XC8H15-4E C8H14-14E S1XC5H9-1E S1XC8H13-17E P8XC8H13-16E P8XC8H13-15E C8H12-137E S6XC10H17-14E S7XC10H17-14E P8XC8H13-14E C8H12-147E S1XC5H7-14E S1XC4H6-3EcC6H11 S7XC10H17-13E P8XC8H13-13E S6XC9H14-13E5M T5XC9H14-13E5M P7XC7H10-13E5M C7H9-136E5M C9H14-135E P6XC6H10-3E4C2H3 S5XC8H14-3E4C2H3 C6H9-13E-3-C2H3 S4XC8H14-1E5C2H3 T5XC8H14-1E5C2H3 P6XC6H10-1E5C2H3 C6H11-1E-3-C2H3 C5H9-1E-2-C2H3 C6H9-15E-2-C2H3 S5XC8H14-1E4C2H3 T4XC8H14-1E4C2H3 P6XC6H10-1E4C2H3 C6H9-15E-3-C2H3 C6H8-15E-3-CH2 C7H12-1E-3-CH2 T4XC7H10CH2C2H5 P5XC5H61ECH2C2H5 C6H8-1E-34-CH2 C2H5C2H3S2XcC6H9 T4XC10H17-46E P1XC8H13-24E T4XC9H15-3E5CH2 S1XC7H11-1E3CH2 C7H10-3-CH2 C4H9T1XcC6H8-2E S1XC6H9-23-CH2 C3H7CH2T1XcC6H8 spiro-4-5-decane CH2-2-CH3cC6H7 S1XC3H4CH3cC6H10 C3H5CH3S6XcC6H10 C3H5CH3S4XcC6H8 C3H5CH3cC6H8-24E C3H5CH3S6XcC6H8 CH2cC5H6 cC5H5-13E2M C2H3C2H3S2XcC5H8 decalin-1b247E decalin-15E

C5H8 T1XcC5H5 T2XC5H9-1E cC5H8 S1XC7H11-13E T3XC6H9-13E T2XC6H9-15E T2XC5H7-14E T2XC6H11-1E C5H6-14E-3-CH2 C8H14-24E P1XC6H11-2E S1XC6H9-15E P6XC6H9-14E S1XC5H6-14E3M P5XC5H7-13E C7H10-1E-34-CH2

!HYD-SPECIES HYD S3X-HYD S8X-HYD T1X-HYD S2X-HYD S7X-HYD INT1A INT2B INT3C INT4D INT5E HYD-6E HYD-7E S9XC9H1515E S9XC9H1517E C2H31C6H10CH2 S3XC9H1518E P1XC2H4C5H71E S4XC9H1518E P1XC3H6C6H915E P1XC4H71E P1XC2H4C7H1216E P9XC9H1515E CH2C3H51EcC5H8 C4H71ES2XcC5H8 HYD-3E HYD-2E P7XC7H1113E C2H4C2H32EcC5H8 P1XC2H4C3H714E HYD-1E S5XcC9H155E P1XCH2-2-cC6H9 P9XC9H1516E P1XC2H4C5H71E CH2P1XC4H8cC5H7 P1XC4H8cC5H71E HYD-6E HYD-16E HYD-5E CH2ECH2cC5H7 P1XC3H6cC6H9 CH2S2XcC6H9 P1XC3H6cC6H9 P1XCH2-1-cC6H9 T6X-HYD-1E CH21ES2XcC6H71E CH21ECH21EcC5H6 T1X-HYD-2E S1XCH21EC6H73E P1XC4H63EcC5H71E P1XC3H6C6H715E C2H4CH21EcC6H7 P1XMCH-15E S6X-HYD-16E S2X-HYD-16E P1XCH2C2H3cC6H8 HYD-7E C2H4C2H31EcC5H8 C2H5C2H31EcC5H8 CH3C2H31EcC6H10 CH2C2H51EcC6H9 C3H51EcC6H11 T6X-HYD-7E P1XC4H8cC5H514E C3H6CH2EC5H5E T1X-HYD-6E P1XC2H3CH2cC6H9 P1XC3H6CH2cC5H5 CH2CH21EcC5H51E C4H71EcC5H9 CH3C3H51EcC5H8 CH21EC3H7cC5H7 P1XC2H21EcC5H71E P1XC3H4EcC6H9E CH2CH21EcC5H5-2E aC3H5 S3XC5H7-14E C3H61ES1XC6H9 P1XC3H6C6H915E S9XC9H1514E S7XC7H11-14E C5H814E P1XC2H3C7H1216E P1XC2H4cC5H71E S5XcC9H151E P1XC4H8cC5H7-2E P1XC2H4cC5H72E P1XC3H6cC6H715E CH2ES2XcC6H75E C3H6CH2EcC5H5E P1XC2H4cC5H514E

C2H4CH21EcC6H9 CH21EC2H4cC6H73E CH2C2H31EcC6H10 C3H61ES1XcC6H10 P1XCH2C6H915E C3H5CH21EcC5H6 T1X-HYD-7E PXC2H4C2H3cC5H6 S1XC2H3cC5H6-1E C2H3T2XcC5H6

P7XC4H8C5H714E P5XC2H4C5H714E P7XC7H11-15E P1XC3H6C4H513E

T2XC7H11-16E T1XC7H11-16E S3XC7H11-15E S4XC7H11-16E

!AR argon !N2 nitrogen !HE helium !H H atom !H2 hydrogen !H2O water !O2 oxygen !CH methylidene, doublet !CH* methylidene, singal !CH2 methylene, triplet B(1) !CH2* methylene, singlet A(1) !CH3 methyl radical, doublet !CH4 methane !CO carbon monoxide !CO2 carbon dioxide !C2H ethynyl !C2H2 acetylene !H2CC vinylidene !C2H3 vinyl !C2H4 ethylene !C2H5 ethyl !C2H6 ethane !C3H2 propargylene, HCCCH !C3H3 propargyl, CH2CCH !aC3H4 allene !pC3H4 propyne !aC3H5 allyl !CH3CCH2 propen-2-yl / CH2=C*-CH3 !CH3CHCH propenyl (E and Z) / *CH=CH-CH3 !C3H6 propene !nC3H7 n-propyl / *CH2-CH2-CH3 !iC3H7 isopropyl / CH3-CH*-CH3 !C3H8 propane !C4H butadiynyl/ CHCCC !C4H2 1,3-butadiyne !nC4H3 *CH=CH-CCH, but-1-en-3-ynyl !iC4H3 CH2C*-CCH !C4H4 1-buten-3-yne !nC4H5 *CH=CH-CH=CH2 !iC4H5 CH2=C*-CH=CH2 !C4H5-2 CH3-CC-*CH2 !C4H6 1,3-butadiene !C4H612 1,2-butadiene !C4H6-2 2-butyne !C5H8 1-pentyne !C4H7 CH2*-CH2-CH=CH2 !SAXC4H7 CH3-CH*-CH=CH2 !iC4H7 CH2=C(CH3)CH2* !C4H7-2 CH3-CH*-CH=CH2 !iC4H8 CH2=C(CH3)2 !C4H8-1 CH2=CH-CH2-CH3 !C4H8-2 CH3-CH=CH-CH3

REACTIONS

CH reactions

CH+H = C+H2 1.100E+14 0.000 0.00 ! GRI CH+H2 = CH2+H 1.107E+08 1.790 1670.00 ! GRI

CH2(triplet) reactions

CH2+H(+M) = CH3(+M) 2.500E+16 -0.800 0.00 ! GRI LOW / 3.200E+27 -3.140 1230.00/ TROE/ 0.6800 78.00 1995.0 5590.0 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ CH2+H2 = H+CH3 5.000E+05 2.000 7230.00 ! GRI CH2+C = C2H+H 5.000E+13 0.000 0.00 ! GRI CH2+CH = C2H2+H 4.000E+13 0.000 0.00 ! GRI CH2+CH2 = C2H2+H2 3.200E+13 0.000 0.00 ! GRI

CH2(singlet) reactions

CH2*+AR = CH2+AR 9.000E+12 0.000 600.00 ! GRI CH2*+H = CH+H2 3.000E+13 0.000 0.00 ! GRI CH2*+H2 = CH3+H 7.000E+13 0.000 0.00 ! GRI

CH3

CH3+H(+M) = CH4(+M) 1.270E+16 -0.630 383.00 ! GRI LOW / 2.477E+33 -4.760 2440.00 / TROE/ 0.7830 74.00 2941.00 6964.0 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ CH3+C = C2H2+H 5.000E+13 0.000 0.00 ! GRI CH3+CH = C2H3+H 3.000E+13 0.000 0.00 ! GRI CH3+CH2 = C2H4+H 4.000E+13 0.000 0.00 ! GRI CH3+CH2* = C2H4+H 1.200E+13 0.000 -570.00 ! GRI CH3+CH3(+M) = C2H6(+M) 2.120E+16 -0.970 620.00 ! GRI LOW / 1.770E+50 -9.670

6220.00/ TROE/ 0.5325 151.0 1038.00 4970.0 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ CH3+CH3 = H+C2H5 4.990E+12 0.100 10600.00 ! GRI CH3+C2H = C3H3+H 2.41E+13 0.0 0.0 ! 1986 TSA/HAM

CH4+H = CH3+H2 6.600E+08 1.620 10840.00 ! GRI CH4+CH = C2H4+H 6.000E+13 0.000 0.00 ! GRI CH4+CH2 = CH3+CH3 2.460E+06 2.000 8270.00 ! GRI CH4+CH2* = CH3+CH3 1.600E+13 0.000 -570.00 ! GRI CH4+C2H = C2H2+CH3 1.810E+12 0.0 500.0 ! 1986 TSA/HAM

C2H reactions

C2H+H(+M) = C2H2(+M) 1.000E+17 -1.000 0.00 ! GRI LOW / 3.750E+33 -4.800 1900.00/ TROE/ 0.6464 132.00 1315.00 5566.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H+H2 = H+C2H2 4.900E+05 2.500 560.00 ! GRI

C2H2 reactions

C2H2 (+M) = H2CC (+M) 8.000E+14 -0.520 50750.00 ! 1999 Laskinang LOW / 2.450E+15 -0.640 49700.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/C2H2/2.5/ C2H4/2.5/ C2H3 (+M) = C2H2+H (+M) 3.860E+08 1.620 37048.2 ! 1996 KnyazevSlagle LOW / 2.565E+27 -3.400 35798.72/ TROE/ 1.9816 5383.7 4.2932 -0.0795 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/C2H2/3.00/ C2H4/3.00/

Vinylidene reactions

H2CC+H = C2H2+H 1.000E+14 0.000 0.00 ! USC Mech V2.0 Estimated

C2H3 reactions

C2H3+H(+M) = C2H4(+M) 6.080E+12 0.270 280.00 ! GRI1.2 LOW / 1.400E+30 -3.860 3320.00/ TROE/ 0.7820 207.50 2663.00 6095.00/ H2/2.0/ CH4/2.0/ C2H6/3.0/AR/0.7/ C2H2/3.00/ C2H4/3.00/ C2H3+H = C2H2+H2 9.000E+13 0.000 0.00 ! 1986 TSA/HAM C2H3+H = H2CC+H2 6.000E+13 0.000 0.00 ! USC Mech V2.0 Estimated C2H3+CH3 = C2H2+CH4 3.920E+11 0.000 0.00 ! 1986 TSA/HAM C2H3+C2H3 = C2H2+C2H4 9.600E+11 0.00 0. ! NIST Database

C2H4 reactions

C2H4+H(+M) = C2H5(+M) 1.367E+09 1.463 1355.00 !04-MIL-KLI LOW / 2.027E+39 -6.642 5769.00 / TROE / -0.569 299.0 9147.0 -152.40 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H4(+M)=H2+C2H2(+M) 8.00E+12 0.44 88770. ! GRI3.0 LOW / 1.58E+51 -9.30 97800./ TROE / 0.7345 180 1035 5417/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H4+H = C2H3+H2 5.070E+07 1.900 12950.00 ! 1996 Knyazev et al. C2H4+CH = aC3H4+H 3.000E+13 0.000 0.00 ! USC Mech V2.0 Estimated C2H4+CH = pC3H4+H 3.000E+13 0.000 0.00 ! USC Mech

V2.0 Estimated C2H4+CH2 = aC3H5+H 2.000E+13 0.000 6000.00 ! USC Mech V2.0 Estimated C2H4+CH2* = H2CC+CH4 5.000E+13 0.000 0.00 ! USC Mech V2.0 Estimated C2H4+CH2* = aC3H5+H 5.000E+13 0.000 0.00 ! USC Mech V2.0 Estimated C2H4+CH3 = C2H3+CH4 2.270E+05 2.000 9200.00 ! GRI C2H4+C2H = C4H4+H 1.200E+13 0.000 0.00 ! 1986 TSA/HAM

C2H5 reactions

C2H5+H(+M) = C2H6(+M) 5.210E+17 -0.990 1580.00 ! GRI LOW / 1.990E+41 -7.080 6685.00/ TROE / 0.8422 125.0 2219.00 6882.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H5+H = C2H4+H2 2.000E+12 0.000 0.00 ! GRI C2H5+CH3(+M) = C3H8(+M) 4.90E+14 -0.50 0.0 ! 1988 TSA LOW / 6.80E+61 -13.42 6000.0/ TROE / 1.000 1000.0 1433.9 5328.8 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H6 reactions

C2H6+H = C2H5+H2 1.15E+08 1.900 7530.00 ! GRI C2H6+CH2* = C2H5+CH3 4.00E+13 0.000 -550.00 ! GRI C2H6+CH3 = C2H5+CH4 6.14E+06 1.740 10450.00 ! GRI C2H6+C2H=C2H2+C2H5 3.61E+12 0.00 0 ! 1986 TSA/HAM C2H6+C2H3=C2H4+C2H5 6.01E+02 3.30 10502 ! 1986 TSA/HAM

C3H2 reactions

C3H2+H(+M)=C3H3(+M) 1.02e+13 0.27 279.64 ! 2009 Blanquart et al. LOW/ 2.80e+30 -3.860 3319.79/ TROE/ 0.782 207.50 2663.00 6095.00/ H2/2.00/ AR/0.70/CH4/2.00/ C2H6/3.00/ C3H2+CH=C4H2+H 5.00E+13 0.0 0. ! USC Mech V2.0

C3H3 reactions

C3H3+H = C3H2+H2 1.00E+13 0.0 1000. ! USC Mech V2.0 C2H2+CH2 = C3H3+H 1.20E+13 0.00 6620.00 ! 1988 Bohland et al.; 1988 Frank et al. C2H2+CH2* = C3H3+H 2.00E+13 0.00 0.00 ! 1997 WangFrenklach

C3H4 reactions

! aC3H4=pC3H4 6.0256E+53 -12.18 84276. ! J. A. Miller Mechanism ! PLOG /0.03947 6.0256E+53 -12.18 84276./ ! PLOG /1. 7.7625E+39 -7.80 78446./ ! PLOG /10. 4.7863E+48 -10.0 88685./ C3H3+H=pC3H4 3.6308E+36 -7.36 6039. ! J. A. Miller Mechanism PLOG /0.03947 3.6308E+36 -7.36 6039./ PLOG /1. 7.943E+29 -5.06 4861./ PLOG /10. 1.072E24 -3.15 3261./ C3H3+H=aC3H4 3.3884E+36 -7.41 6337. ! J. A. Miller Mechanism PLOG /0.03947 3.3884E+36 -7.41 6337./ PLOG /1. 3.1623E+29 -5. 4711./ PLOG /10. 8.7096E+23 -3.20 3255./ aC3H4+H = C3H3+H2 6.60E+03 3.1 5522 ! 2008 Miller 30 Torr aC3H4+CH3=C3H3+CH4 6.600E-4 5.000

8300 ! 2009 Kiefer et al. H+aC3H4 = H+pC3H4 1.47E+13 0.26 4103 ! 2008 Miller 30 Torr aC3H4+C2H = C2H2+C3H3 1.00E+13 0.0 0.0 ! 1997 WangFrenklach ! H+aC3H4 = CH3+C2H2 2.72E+09 1.2 6834 ! 2008 Miller 30 Torr pC3H4+H = C3H3+H2 3.57E+04 2.8 4821 ! 2008 Miller 30 Torr ! pC3H4+CH3=C3H3+CH4 2.200E-4 5.000 8300 ! 2009 Kiefer et al. pC3H4+C3H3 = aC3H4+C3H3 6.14E+06 1.74 10450. ! USC Mech V2.0 Estimated pC3H4+C2H = C2H2+C3H3 1.00E+13 0.0 0.0 ! USC Mech V2.0 Estimated ! H+pC3H4 = C2H2+CH3 3.89E+10 0.989 4114 ! 2008 Miller 30 Torr C2H2+CH3 = pC3H4+H 2.51E+11 0.56 11453.0 !99DAV/LAW RRKM !99DAV/LAW RRKM ! activatin energy decrease 4 kcal/mol in this work ! PLOG / 0.1 4.50E+06 1.86 11600.0 / !99DAV/LAW RRKM 0.1 atm ! PLOG / 1 2.56E+09 1.10 13644.0 / !99DAV/LAW RRKM 1 atm ! PLOG / 2 2.07E+10 0.85 14415.0 / !99DAV/LAW RRKM 2 atm ! PLOG /5 2.51E+11 0.56 15453.0 / !99DAV/LAW RRKM 5 atm ! PLOG /10 1.10E+12 0.39 16200.0 / !99DAV/LAW RRKM 10 atm ! PLOG /100 2.10E+12 0.37 18100.0 / !99DAV/LAW RRKM 100 atm C2H2+CH3 = aC3H4+H 2.40E+09 0.91 20700.0 ! ! PLOG /0.1 2.40E+09 0.91 20700.0 / !99DAV/LAW RRKM 0.1 atm ! PLOG /1 5.14E+09 0.86 22153.0 / !99DAV/LAW RRKM 1 atm ! PLOG /2 1.33E+10 0.75 22811.0 / !99DAV/LAW RRKM 2 atm ! PLOG /5 9.20E+10 0.54 23950.0 / !99DAV/LAW RRKM 5 atm ! PLOG /10 5.10E+11 0.35 25000.0 / !99DAV/LAW RRKM 10 atm ! PLOG /100 7.30E+12 0.11 28500.0 / !99DAV/LAW RRKM 100 atm pC3H4 = aC3H4 6.40E+61 -14.59 88200.0 !99DAV/LAW RRKM PLOG /0.1 6.40E+61 -14.59 88200.0 / !99DAV/LAW RRKM 0.1 atm PLOG/ 0.4 5.81E+62 -14.63 91211.0 / !99DAV/LAW RRKM 0.4 atm PLOG/ 1.0 5.15E+60 -13.93 91117.0 / !99DAV/LAW RRKM 1 atm PLOG/ 2.0 7.64E+59 -13.59 91817.0 / !99DAV/LAW RRKM 2 atm PLOG/ 5.0 3.12E+58 -13.07 92680.0 / !99DAV/LAW RRKM 5 atm PLOG/ 10.0 1.90E+57 -12.62 93300.0 / !99DAV/LAW RRKM 10 atm PLOG/ 100 1.40E+52 -10.86 95400.0 / !99DAV/LAW RRKM 100 atm

CH3CHCH CH3CCH2 and aC3H5 reactions

CH3CHCH+H = aC3H5+H 1.47E+13 0.26 4103 ! Ref H+aC3H4=H+pC3H4

CH3CCH2+H = pC3H4+H2 3.34E+12 0.00 0.0 ! 1999 Davis et al. CH3CCH2+H = aC3H5+H 1.47E+13 0.26 4103 ! Ref aC3H4+H=pC3H4+H CH3CCH2+CH3 = pC3H4+CH4 1.00E+11 0.00 0.0 ! 1999 Davis et al.

aC3H5+H = aC3H4+H2 9.56E+03 2.80 3291.11 ! 2009 Blanquart et al. aC3H5+CH3 = aC3H4+CH4 1.50E+12 -0.32 -131.0 ! 1991 TSA 3.00E+12/2 C2H5+C2H3 = aC3H5+CH3 8.00E+25 -3.46 11775.0 ! 1986 TSA/HAM RRKM 0.1 atm

aC3H4+H = CH3CHCH 1.10E+30 -6.52 15200.0 ! 1999 Davis et al. RRKM PLOG / 0.039 5.05E+29 -6.52 15200.0 / ! EST 0.1 atm /2 PLOG / 0.1 1.10E+30 -6.52 15200.0 / PLOG / 1.0

5.40E+29 -6.09 16300.0 / PLOG / 10.0 2.60E+31 -6.23 18700.0 / PLOG / 100.0 3.20E+31 -5.88 21500.0 / pC3H4+H = CH3CHCH 1.00E+25 -5.00 1800.0 ! 1999 Davis et al. RRKM PLOG / 0.039 5.0E+24 -5.00 1800.0 / ! EST 0.1 atm /2 PLOG / 0.1 1.00E+25 -5.00 1800.0 / PLOG / 1.0 5.50E+28 -5.74 4300.0 / PLOG / 10.0 1.00E+34 -6.88 8900.0 / PLOG / 100.0 9.70E+37 -7.63 13800.0 /

C2H2+CH3 = CH3CHCH 1.40E+32 -7.14 10000.0 ! 1999 Davis et al. RRKM PLOG / 0.039 7.0E+31 -7.14 10000.0 / ! EST 0.1 atm /2 PLOG / 0.1 1.40E+32 -7.14 10000.0 / PLOG / 1.0 3.20E+35 -7.76 13300.0 / PLOG / 10.0 2.40E+38 -8.21 17100.0 / PLOG / 100.0 1.40E+39 -8.06 20200.0 / aC3H4+H = CH3CCH2 9.20E+38 -8.65 7000.0 ! 1999 Davis et al. RRKM PLOG / 0.039 4.60E+38 -8.65 7000.0 / ! EST 0.1 atm /2 PLOG / 0.1 9.20E+38 -8.65 7000.0 / PLOG / 1.0 9.46E+42 -9.43 11190.0 / PLOG / 2.0 8.47E+43 -9.59 12462.0 / PLOG / 5.0 6.98E+44 -9.70 14032.0 / PLOG / 10.0 1.50E+45 -9.69 15100.0 / PLOG / 100.0 1.80E+43 -8.78 16800.0 / pC3H4+H = CH3CCH2 4.60E+44 -10.21 10200.0 ! 1999 Davis et al. RRKM PLOG / 0.039 2.30E+44 -10.21 10200.0 / ! EST 0.1 atm /2 PLOG / 0.1 4.60E+44 -10.21 10200.0 / PLOG / 1.0 1.66E+47 -10.58 13690.0 / PLOG / 2.0 5.04E+47 -10.61 14707.0 / PLOG / 5.0 9.62E+47 -10.55 15910.0 / PLOG / 10.0 7.00E+47 -10.40 16600.0 / PLOG / 100.0 3.20E+44 -9.11 17400.0 / C2H2+CH3 = CH3CCH2 6.80E+20 -4.16 18000.0 ! 1999 Davis et al. RRKM PLOG / 0.039 3.40E+20 -4.16 18000.0 / ! EST 0.1 atm /2 PLOG / 0.1 6.80E+20 -4.16 18000.0 / PLOG / 1.0 4.99E+22 -4.39 18850.0 / PLOG / 2.0 6.00E+23 -4.60 19571.0 / PLOG / 5.0 7.31E+25 -5.06 21150.0 / PLOG / 10.0 9.30E+27 -5.55 22900.0 / PLOG / 100.0 3.80E+36 -7.58 31300.0 / CH3CCH2 = CH3CHCH 1.60E+44 -12.16 52200.0 ! 1999 Davis et al. RRKM PLOG / 0.039 8.0E+43 -12.16 52200.0 / ! EST 0.1 atm /2 PLOG / 0.1 1.60E+44 -12.16 52200.0 / PLOG / 1.0 1.50E+48 -12.71 53900.0 / PLOG / 10.0 5.10E+52 -13.37 57200.0 / PLOG / 100.0 5.80E+51 -12.43 59200.0 / aC3H5 = CH3CHCH 1.30E+55 -14.53 73800.0 ! 1999 Davis et al. RRKM PLOG / 0.039 6.50E+54 -14.53 73800.0 / ! EST 0.1 atm /2 PLOG / 0.1 1.30E+55 -14.53 73800.0 / PLOG / 1.0 5.00E+51 -13.02 73300.0 / PLOG / 10.0 9.70E+48 -11.73 73700.0 / PLOG / 100.0 4.86E+44 -9.84 73400.0 / aC3H5 = CH3CCH2 3.90E+59 -15.42 75400.0 ! 1999 Davis et al. RRKM PLOG / 0.039 1.45E+59 -15.42 75400.0 / ! EST 0.1 atm /2 PLOG / 0.1 3.90E+59 -15.42 75400.0 / PLOG / 1.0 7.06E+56 -14.08 75868.0 / PLOG / 2.0 4.80E+55 -13.59 75949.0 / PLOG / 5.0 4.86E+53 -12.81 75883.0 / PLOG / 10.0 6.40E+51 -12.12 75700.0 / PLOG / 100.0 2.80E+43 -9.27 74000.0 / C2H2+CH3=aC3H5 8.2E+53 -13.32 33200. ! 1999 Davis et al. RRKM PLOG /0.039 4.1E+53 -13.32 33200. / ! EST 0.1 atm /2 PLOG /0.1 8.2E+53 -13.32 33200. / PLOG /1.0 2.7E+53 -12.82 35700. / PLOG /10.0 4.4E+49 -11.40 36700. / PLOG /100.0 3.8E+44 -9.63 37600. / pC3H4+H=aC3H5 1.1E+60 -14.56 28100. ! 1999 Davis et al. RRKM PLOG /0.039 5.5E+59 -14.56 28100. / ! EST 0.1 atm /2 PLOG /0.1 1.1E+60 -14.56 28100. / PLOG /1.0

4.9E+60 -14.37 31600. / PLOG /10.0 2.2E+59 -13.61 34900. / PLOG /100.0 1.6E+55 -12.07 37500. / !aC3H4+H=aC3H5 9.60E+61 -14.67 26000.0 ! 1999 Davis et al. RRKM !PLOG / 0.039 4.80E+61 -14.67 26000.0 / ! EST 0.1 atm /2 !PLOG / 0.1 9.60E+61 -14.67 26000.0 / !PLOG / 1.0 1.52E+59 -13.54 26949.0 / !PLOG / 2.0 3.78E+57 -12.98 26785.0 / !PLOG / 5.0 7.34E+54 -12.09 26187.0 / !PLOG / 10.0 2.40E+52 -11.30 25400.0 / !PLOG / 100.0 6.90E+41 -8.06 21300.0 /

aC3H5=aC3H4+H 1.76E+58 -13.715 76013 PLOG / 0.039 8.80E+57 -13.715 76013/ ! 2009 Kiefer et al./2 PLOG / 0.066 2.53E+58 -13.661 76765/ ! 2009 Kiefer et al. PLOG / 0.132 4.34E+58 -13.628 77634/ ! 2009 Kiefer et al. PLOG / 0.197 8.07E+58 -13.645 78292/ ! 2009 Kiefer et al. PLOG / 0.263 1.49E+59 -13.677 78833/ ! 2009 Kiefer et al. PLOG / 1 1.30E+67 -15.61 88301/ ! 2005 Fernandes et al. PLOG / 4 6.80E+64 -14.75 89043/ ! 2005 Fernandes et al. PLOG / 100 1.5E+15 0 63541/ ! 2005 Fernandes et al.

aC3H5+aC3H5 = pC3H4+C3H6 8.43E+10 0.0 -263 !2009 Kifer et al

C3H6 reactions

aC3H5+H(+M) = C3H6(+M) 2.00E+14 0.00 0.0 ! 1991 TSA LOW / 1.33E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C2H3+CH3 (+M) = C3H6(+M) 2.50E+13 0.000 0.00 ! 1986 TSA/HAM LOW / 4.270E+58 -11.940 9769.80 / TROE / 0.175 1340.6 60000.0 10139.8 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/C2H2/3.00/ C2H4/3.00/ C3H6 = H2 + pC3H4 1.18E+95 -23.6 125649 ! 2009 Kiefer et al. C3H6 = H2 + aC3H4 1.18E+95 -23.6 125649 ! ref:C3H6 = H2 + pC3H4 C3H6+H = C2H4+CH3 8.80E+16 -1.05 6461.0 ! 1991 TSA C3H6+H = aC3H5+H2 1.73E+05 2.50 2490.0 ! 1991 TSA C3H6+H = CH3CCH2+H2 4.00E+05 2.50 9790.0 ! 1991 TSA C3H6+H = CH3CHCH+H2 8.04E+05 2.50 12283.0 ! 1991 TSA C3H6+CH3 = aC3H5+CH4 2.20E+00 3.50 5675.0 ! 1991 TSA C3H6+CH3 = CH3CCH2+CH4 8.40E-01 3.50 11660.0 ! 1991 TSA C3H6+CH3 = CH3CHCH+CH4 1.35E+00 3.50 12848.0 ! 1991 TSA C3H6+C2H3 = C4H6+CH3 7.23E+11 0.0 5000.0 ! 1991 TSA

reactions of nC3H7

nC3H7+H(+M) = C3H8(+M) 3.60E+13 0.00 0.0 ! 1988 TSA LOW / 3.01E+48 -9.32 5833.6/ TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C3H6+H(+M) = nC3H7(+M) 1.33E+13 0.00 3260.7 ! 1991 TSA LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ CH3+C2H4(+M)= nC3H7(+M) 2.55E+06 1.600 5700. ! 1988 TSA LOW / 3.00E+63 -14.6 18170./ TROE /0.1894 277. 8748. 7891./ H2/2.00/ CH4/2.00/ C2H6/3.00/ AR/0.70/ nC3H7+H = C2H5+CH3 3.40E+18 -1.33 5386.0 !

1988 TSA nC3H7+H = C3H6+H2 1.80E+12 0.00 0.0 ! 1988 TSA nC3H7+CH3 = CH4+C3H6 1.10E+13 -0.32 0.0 ! 1988 TSA

reactions of iC3H7

iC3H7+H(+M) = C3H8(+M) 2.40E+13 0.00 0.0 ! 1988 TSA LOW / 1.70E+58 -12.08 11263.7/ TROE / 0.649 1213.1 1213.1 13369.7 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C3H6+H(+M) = iC3H7(+M) 1.33E+13 0.00 1559.8 ! 1991 TSA LOW / 8.70E+42 -7.50 4721.8/ TROE / 1.000 1000.0 645.4 6844.3/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/ iC3H7+H = CH3+C2H5 5.90E+23 -2.81 10009.0 ! 1988 TSA RRKM 0.1 atm iC3H7+H = C3H6+H2 3.20E+12 0.00 0.0 ! 1988 TSA iC3H7+CH3 = CH4 + C3H6 9.4E+10 0.68 0.0 ! 1988 TSA

reactions of C3H8

C3H8+H = H2+nC3H7 1.30E+06 2.54 6756.0 ! 1988 TSA C3H8+H = H2+iC3H7 1.30E+06 2.40 4471.0 ! 1988 TSA C3H8+CH3 = CH4+nC3H7 9.03E-01 3.65 7153.0 ! 1988 TSA C3H8+CH3 = CH4+iC3H7 1.51E+00 3.46 5480.0 ! 1988 TSA

reactions of C4H2

C2H2+C2H2 = C4H2+H2 1.50E+13 0.0 42700 ! 2007 Gueniche et al. C2H2+C2H = C4H2+H 9.60E+13 0.00 0.00 ! 1991 SHI/MIC, 1992 Koshi et al., 1993 Fahrat et al.

reactions of nC4H3

C2H2+C2H(+M) = nC4H3(+M) 8.30E+10 0.899 -363.00 ! 1992 Wang LOW / 1.240E+31 -4.718 1871.00/ TROE / 1.0 100. 5613. 13387./ H2/2.0/ CH4/2.0/ C2H6/3.0/ C2H2/2.5/ C2H4/2.5/ nC4H3 + H = C4H4 1.10E+42 -9.65 7000.0 ! 1997 WangFrenklach PLOG / 0.026 1.10E+42 -9.65 7000.0/ PLOG / 0.118 1.10E+42 -9.65 7000.0/ PLOG / 1.0 2.00E+47 -10.26 13070.0/ C4H2 + H = nC4H3 1.70E+49 -11.67 12804.0 ! 1997 WangFrenklach PLOG / 0.026 1.70E+49 -11.67 12804.0/ PLOG / 0.118 3.30E+50 -11.80 15010.0/ PLOG / 1.0 1.10E+42 -8.72 15300.0/ nC4H3 = iC4H3 3.70E+61 -15.81 54890.0 ! 1997 WangFrenklach PLOG / 0.026 3.70E+61 -15.81 54890.0/ PLOG / 0.118 1.00E+51 -12.45 51000.0/ PLOG / 1.0 4.10E+43 -9.49 53000.0/ C3H3+CH = nC4H3+H 5.00E+13 0.0 0.0 ! USC Mech V2.0 Estimated C3H2+CH2 = nC4H3+H 5.00E+13 0.0 0.0 ! 1992 MillerMelius nC4H3+H = C4H2+H2 3.00E+13 0.00 0.0 ! = 0.5*C2H3+H USC Mech V2.0 nC4H3 + H = C2H2 + H2CC 1.60E+19 -1.60 2220.0 ! 1997 WangFrenklach 0.026 atm RRKM nC4H3 + H = iC4H3 + H 2.40E+11 0.79 2410.0 ! 1997 WangFrenklach 0.026 atm RRKM

reactions of iC4H3

C2H2+C2H(+M) = iC4H3(+M) 8.30E+10 0.899 -363.00 ! 1992 Wang LOW / 1.240E+31 -4.718 1871.00/ TROE / 1.0 100. 5613. 13387./ H2/2.0/ CH4/2.0/ C2H6/3.0/C2H2/2.5/ C2H4/2.5/ C4H2+H(+M)=iC4H3(+M) 4.31E+10 1.160 1751.91 ! 1992 Wang LOW / 2.30e+45 -8.100 2507.17/ TROE / 0.0748 1.00 -4216.00/ H2/2.00/ AR/0.70/ CH4/2.00/ C2H6/3.00/ iC4H3 + H = C4H4 4.20E+44 -10.27 7890.0 ! 1997 WangFrenklach PLOG / 0.026 4.20E+44 -10.27 7890.0 / PLOG / 0.118 5.30E+46 -10.68 9270.0 / PLOG / 1.0 3.40E+43 -9.01 12120.0/ iC4H3+H = C2H2+H2CC 2.40E+19 -1.60 2800.0 ! 1997 WangFrenklach 0.026 atm RRKM iC4H3+H = C4H2+H2 6.00E+13 0.00 0.0 ! = C2H3+H USC Mech V2.0 C3H3+CH = iC4H3+H 5.00E+13 0.0 0.0 ! USC Mech V2.0 Estimated

reactions of C4H4

H2CC+C2H2(+M) = C4H4(+M) 3.50E+05 2.055 -2400. ! 1999 LaskinWang LOW / 1.40E+60 -12.599 7417./ TROE / 0.98 560. 580. 4164./ H2/2.0/ CH4/2.0/ C2H2/3.0/ C2H4/3.0/ C2H6/3.0/ C2H3+C2H = C4H4 1.00E+14 0.00 0.0 ! 1988 Duran et al. C3H3+CH2* = C4H4+H 4.00E+13 0.0 0.0 ! 2007 Gueniche et al. C4H4+H = nC4H3+H2 6.65E+05 2.53 12240. ! 1997 WangFrenklach C4H4+H = iC4H3+H2 3.33E+05 2.53 9240. ! 1997 WangFrenklach C2H3+C2H2=C4H4+H 5.00E+14 -0.71 6700. ! 1997 WangFrenklach 0.026 atm RRKM C3H3+CH2=C4H4+H 5.00E+13 0.00 0.0 ! 1992 MillerMelius C3H2+CH3=C4H4+H 5.00E+12 0.00 0.0 ! USC Mech V2.0

reactions of nC4H5

C2H3 + C2H2 = nC4H5 1.10E+31 -7.14 5600. ! 1997 WangFrenklach PLOG / 0.013 1.10E+31 -7.14 5600. / PLOG / 0.026 1.10E+32 -7.33 6200. / PLOG / 0.118 2.40E+31 -6.95 5600. / PLOG / 1.0 9.30E+38 -8.76 12000./ PLOG / 10.0 8.10E+37 -8.09 13400./ C4H4 + H = nC4H5 1.20E+51 -12.57 12300. ! 1997 WangFrenklach PLOG / 0.013 1.20E+51 -12.57 12300./ PLOG / 0.026 4.20E+50 -12.34 12500./ PLOG / 0.118 1.10E+50 -11.94 13400./ PLOG / 1.0 1.30E+51 -11.92 16500./ PLOG / 10.0 6.20E+45 -10.08 15800./ nC4H5 = iC4H5 2.40E+60 -16.08 47500. ! 1997 WangFrenklach PLOG / 0.013 2.40E+60 -16.08 47500./ PLOG / 0.026 1.30E+62 -16.38 49600./ PLOG / 0.118 4.90E+66 -17.26 55400./ PLOG / 1.0 1.50E+67 -16.89 59100./ PLOG / 10.0 2.00E+60 -14.46 58600./ nC4H5+H = iC4H5+H 1.00E+36 -6.26 17486. ! 1997 WangFrenklach 0.026 atm RRKM C2H3+C2H3 = nC4H5+H 1.10E+24 -3.28 12395. ! 1997 WangFrenklach 0.026 atm RRKM nC4H5+H = C4H4+H2 1.50E+13 0.00 0.0 ! 1997 WangFrenklach

reactions of iC4H5

C2H3 + C2H2 = iC4H5 5.00E+34 -8.42 7900. ! 1997 WangFrenklach PLOG / 0.013 5.00E+34 -8.42 7900. / PLOG / 0.026 2.10E+36 -8.78 9100. / PLOG / 0.118 1.00E+37 -8.77 9800. / PLOG / 1.0 1.60E+46 -10.98 18600./ PLOG / 10.0 5.10E+53 -12.64 28800./ C4H4 + H = iC4H5

6.10E+53 -13.19 14200. ! 1997 WangFrenklach PLOG / 0.013 6.10E+53 -13.19 14200./ PLOG / 0.026 9.60E+52 -12.85 14300./ PLOG / 0.118 2.10E+52 -12.44 15500./ PLOG / 1.0 4.90E+51 -11.92 17700./ PLOG / 10.0 1.50E+48 -10.58 18800./ C2H3+C2H3 = iC4H5+H 1.50E+30 -4.95 12958. ! 1997 WangFrenklach 0.026 atm RRKM iC4H5+H = C4H4+H2 3.0E+13 0.00 0. ! 1997 WangFrenklach iC4H5+H=C3H3+CH3 1.0E14 0.00 0. ! 2009 Hansen et al C3H4 FLAME

reactions of C4H5-2

C4H5-2 = iC4H5 1.30E+62 -16.38 49600. ! nC4H5=¿iC4H5 1997 WangFrenklach 0.026 atm RRKM iC4H5+H = C4H5-2+H 1.00E+36 -6.26 17486. ! = nC4H5+H=¿iC4H5+H 0.026 atm RRKM 1997 WangFrenklach

Ractions of c-C4H5

c-C4H5 + H = C4H6 1.000E+13 0.000 0.00 ! Est. HW, fast c-C4H6 -¿ C4H6 - Lifshitz USC Mech V2.0 c-C4H5 + H = C2H4 + C2H2 1.000E+13 0.000 0.00 ! Est. HW USC Mech V2.0 c-C4H5 = C4H4 + H 3.000E+12 0.000 52000.00 ! Est. HW USC Mech V2.0 c-C4H5 = C2H3 + C2H2 2.000E+12 0.000 58000.00 ! Est. HW USC Mech V2.0

reactions of C4H6

C4H6 = C4H4+H2 8.33E+13 0.0 94700. ! PLOG / 0.039 8.33E+13 0.0 94700./ ! EST 2.5E+15 /30 PLOG / 1.0 2.50E+15 0.0 94700./ ! 1996 Hidaka et al. C4H6 = H2CC+C2H4 1.00E+13 0.0 85000.0 ! EST C2H3 + C2H3 = C4H6 7.00E+57 -13.82 17629. ! 1997 WangFrenklach PLOG / 0.026 7.00E+57 -13.82 17629./ PLOG / 0.118 1.50E+52 -11.97 16056./ PLOG / 1.0 1.50E+42 -8.84 12483./ C4H6 = iC4H5 + H 8.20E+51 -10.92 118409. ! 1997 WangFrenklach PLOG / 0.026 8.20E+51 -10.92 118409./ PLOG / 0.118 3.30E+45 -8.95 115934./ PLOG / 1.0 5.70E+36 -6.27 112353./ C4H6 = nC4H5 + H 3.50E+61 -13.87 129677. ! 1997 WangFrenklach PLOG / 0.026 3.50E+61 -13.87 129677./ PLOG / 0.118 8.50E+54 -11.78 127472./ PLOG / 1.0 5.30E+44 -8.62 123608./ C4H6+H = nC4H5+H2 1.33E+06 2.53 12240. ! =C2H4+H USC Mech V2.0 C4H6+H = iC4H5+H2 6.65E+05 2.53 9240. ! USC Mech V2.0 Estimated C4H6+H = C2H4+C2H3 1.46E+30 -4.34 21647. ! USC Mech II (1997 WangFrenklach 1 atm) C4H6+H = pC3H4+CH3 2.00E+12 0.0 7000. ! USC Mech V2.0 Estimated C4H6+H = aC3H4+CH3 2.00E+12 0.0 7000. ! USC Mech V2.0 Estimated C4H6+CH3 = nC4H5+CH4 2.00E+14 0.0 22800. ! 1996 Hidaka et al. C4H6+CH3 = iC4H5+CH4 1.00E+14 0.0 19800. ! 1996 Hidaka et al. C4H6+C2H3 = nC4H5+C2H4 5.00E+13 0.0 22800. ! 1996 Hidaka et al. C4H6+C2H3 = iC4H5+C2H4 2.50E+13 0.0 19800. ! 1996 Hidaka et al. C4H6+C3H3 = nC4H5+aC3H4 1.00E+13 0.0 22500. ! 1996 Hidaka et al. C4H6+C3H3 = iC4H5+aC3H4 0.50E+13 0.0 19500. ! 1996 Hidaka et al. C4H6+aC3H5 = nC4H5+C3H6

1.00E+13 0.0 22500. ! USC Mech V2.0 Estimated C4H6+aC3H5 = iC4H5+C3H6 0.50E+13 0.0 19500. ! USC Mech V2.0 Estimated

reactions of 1,2-C4H6

C4H612 = C4H6 1.00E+12 0.0 65000 ! PLOG / 0.039 1.00E+12 0.0 65000/ ! EST 3.00E+13 /30 PLOG / 1.0 3.00E+13 0.0 65000/ ! 1996 Hidaka et al

C3H3+CH3 (+M) = C4H612 (+M) 1.50E+12 0.0 0.0 ! 1997 WangFrenklach LOW / 2.60E+57 -11.94 9770.0/ TROE / 0.175 1340.6 60000.0 9769.8 / H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C4H612+H = nC4H5+H2 1.33E+06 2.53 12240. ! = C2H4+H C4H612 = iC4H5+H 2.10E+14 0.0 92600. ! PLOG / 0.039 2.10E+14 0.0 92600./ ! EST 4.20E+15 /20 PLOG / 1.0 4.20E+15 0.0 92600./ ! 1995 Leung et al. C4H612+H = C4H6+H 2.00E+13 0.0 4000. ! USC Mech V2.0 Estimated C4H612+H = iC4H5+H2 1.70E+05 2.5 2490. ! = C3H6+H USC Mech V2.0 C4H612+H = aC3H4+CH3 2.00E+13 0.0 2000. ! 1997 WangFrenklach C4H612+H = pC3H4+CH3 2.00E+13 0.0 2000. ! 1997 WangFrenklach C4H612+CH3 = iC4H5+CH4 7.00E+13 0.0 18500. ! 1988 Kern et al. reactions of C4H6-2

C4H6-2 = C4H6 1.00E+12 0.000 65000. ! PLOG / 0.039 1.00E+12 0.000 65000./ ! EST 3.00E+13 /30 PLOG / 1.0 3.00E+13 0.000 65000./ ! 1996 Hidaka et al. C4H6-2 = C4H612 1.00E+12 0.000 67000. ! PLOG / 0.039 1.00E+12 0.000 67000./ ! EST 3.00E+13 /30 PLOG / 1.0 3.00E+13 0.000 67000./ ! 1996 Hidaka et al. C4H6-2+H = C4H612+H 2.00E+13 0.0 4000. ! USC Mech V2.0 Estimated C4H6-2+H = C4H5-2+H2 3.40E+05 2.5 2490. ! = C3H6+H USC Mech V2.0 C4H6-2+H = CH3+pC3H4 2.60E+5 2.500 1000. ! 1996 Hidaka et al. C4H6-2 = H+C4H5-2 1.67E+14 0.000 87300. ! PLOG / 0.039 1.67E+14 0.000 87300./ ! EST 5.00E+15 /30 PLOG / 1.0 5.00E+15 0.000 87300./ ! 1996 Hidaka et al. C4H6-2+CH3 = C4H5-2+CH4 1.40E+14 0.0 18500. ! USC Mech V2.0 Estimated

reactions of saxC4H7

SAXC4H7(+M) = C4H6+H(+M) 4.70E+08 1.32 44697.6 ! JetSurF 2.0 LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ SAXC4H7+H = C4H612+H2 1.80E+13 0.0 0.0 ! EST JetSurF 2.0 C4H612+H = SAXC4H7 1.20E+10 0.69 3000 ! 2007 Gueniche et al./10 SAXC4H7+H = C4H6+H2 1.80E+13 0.00 0.0 ! (aC3H5+H) JetSurF 2.0 SAXC4H7+CH3=C4H6+CH4 3.00E+12 -0.32 -131.0 ! aC3H5+CH3 = aC3H4+CH4 JetSurF 2.0 SAXC4H7+CH3 = C4H612+CH4 1.00E+13 0.00 0.0 ! EST JetSurF 2.0 SAXC4H7+C2H3 = C4H6+C2H4 1.00E+13 0.00 0.0 ! EST JetSurF 2.0 SAXC4H7+C2H3 = C4H612+C2H4 1.00E+13 0.00 0.0 ! EST JetSurF 2.0

reactions of C4H7

C4H7 = C4H6+H 1.27E+24 -4.75 23777 ! PLOG / 0.033 1.27E+24 -4.75 23777 / ! 2009 Kiefer et al. PLOG / 0.066 1.38E+26 -5.221 25729 / ! 2009 Kiefer et al. PLOG / 0.132 1.75E+28 -5.709 27764 / ! 2009 Kiefer et al. PLOG / 0.197 3.16E+29 -6.003 28985 / ! 2009 Kiefer et al. PLOG / 0.263 2.69E+30 -6.222 29890 / ! 2009 Kiefer et al. PLOG / 1.0 2.48E+53 -12.30 52000 / ! 1997 WangFrenklach PLOG / 10 1.85E+48 -10.50 51770 / ! 1997 WangFrenklach C2H4+C2H3 = C4H7 1.23E+35 -7.76 9930.0 ! 1997 WangFrenklach PLOG / 0.039 6.15E+34 -7.76 9930.0 / ! EST 0.1 atm/2 PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/ C4H7+H = SAXC4H7+H 1.00E+13 0.00 0.0 ! EST JetSurF 2.0 C4H7+H = CH3+aC3H5 2.00E+21 -2.00 11000.0 ! Estimated USC Mech V2.0 C4H7+H = C4H6+H2 1.80E+12 0.00 0.0 ! = nC3H7+H USC Mech V2.0 C4H7+CH3 = C4H6+CH4 1.10E+13 0.00 0.0 ! = nC3H7+CH3 USC Mech V2.0

reactions of C4H7-2 CH3CCHCH3

C4H7-2 = SAXC4H7 2.00E+12 0.0 47000 ! 2007 Gueniche et al./10 C4H7-2 = CH3+aC3H4 2.00E+12 0.0 32500 ! 2007 Gueniche et al./10 C4H7-2 = C4H7 3.30E+08 1.0 43300 ! 2007 Gueniche et al./10 C4H612+H = C4H7-2 1.30E+12 0.0 3200 ! 2007 Gueniche et al./10 CH3CCHCH3=pC3H4+CH3 2.00E+12 0.0 31500 ! 2007 Gueniche et al./10 C4H7-2+H=pC3H4+CH4 3.00E+13 0.0 0.0 ! EST

reactions of iC4H7 iC4H7-1

iC4H7=aC3H4+CH3 1.00E+12 0.0 51000 ! 2009 Yasunaga et al. /10 iC4H7+H=aC3H4+CH4 6.31E+13 0.0 0.0 ! 2009 Yasunaga et al. iC4H7=SAXC4H7 6.00E+13 0. 70000 ! 2012 Zhang et al. iC4H7+H=SAXC4H7+H 1.47E+13 0.26 4103 ! Ref aC3H4+H=pC3H4+H iC4H7+H = aC3H5+CH3 2.20E+51 -9.98 37730.0 ! =(aC3H5+H) TS5 0.1 atm USC Mech V2.0 iC4H7+H = CH3CCH2+CH3 2.20E+51 -9.98 37730.0 ! =(aC3H5+H) TS5 0.1 atm USC Mech V2.0 iC4H7-1=pC3H4+CH3 1.30E+14 0.0 37000 ! 2009 Yasunaga et al. iC4H7-1=iC4H7 5.00E+12 0.0 36000 ! 2009 Yasunaga et al. reactions of C4H8-1

aC3H5+CH3(+M)=C4H8-1(+M) 1.00E+14 -0.32 -262. ! 1991 TSA LOW /3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H5+C2H3(+M) = C4H8-1(+M) 1.50E+13 0.00 0.0 ! 1986 TSA/HAM LOW / 1.55E+56 -11.79 8984.5/ TROE / 0.198 2277.9 60000.0 5723.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C4H7+H(+M) = C4H8-1(+M) 3.60E+13 0.00 0.0 ! = nC3H7+H USC Mech V2.0 LOW / 3.01E+48 -9.32 5833.6/ TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ SAXC4H7+H(+M) = C4H8-1(+M) 2.00E+14 0.00 0.0 ! (ac3H5+H) JetSurF 2.0 LOW / 2.66E+60 -12.00 5967.8 / ! 2*(aC3H5+H) H2/2/ CH4/2/ C2H6/3/ C4H8-1+H=C4H8-2+H 5.00E+14 -0.26 7600.0 ! Ref: pC3H4+H = aC3H4+H in USC Mech V2.0 C4H7-2+H = C4H8-1 1.00E+13 0.0 0.0 ! EST 2012 Zhang et al.

C4H8-1+H = SAXC4H7+H2 1.30E+06 3.40 4471.0 ! (C3H8+H) USC Mech V2.0 !!ori n=2.40 C4H8-1+H = C4H7+H2 6.50E+05 2.5 6756 ! Ref C6H12-1E+H=P6XC6H11-1E+H2 in 2009 Kiefer et al. C4H8-1+H = C4H7-2+H2 4.00E+05 2.50 9790.0 ! Ref to C3H6+H = CH3CCH2+H2 C4H8-1+H = C3H6+CH3 3.20E+22 -2.39 11180 ! 2012 Zhang et al. C4H8-1+H = C2H4+C2H5 8.80E+16 -1.05 6461.0 ! Ref C3H6+H = C2H4+CH3 C4H8-1+CH3 = SAXC4H7+CH4 2.82E+00 3.60 7153 ! Ref C6H12-1E+CH3=S3XC6H11-1E+CH4 in 2009 Kiefer et al. C4H8-1+CH3 = C4H7+CH4 4.50E-01 3.65 7153.0 ! (C3H8+CH3) USC Mech V2.0

reactions of C4H8-2

CH3CHCH+CH3(+M) = C4H8-2(+M) 5.00E+13 0.0 0.00 ! Ref to C2H3+CH3(+M)=C3H6(+M) LOW / 8.54E+58 -11.940 9769.80/ TROE / 0.175 1340.6 60000.0 10139.8/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/C2H2/3.00/ C2H4/3.00/ SAXC4H7+H(+M) = C4H8-2(+M) 2.00E+14 0.00 0.0 ! (ac3H5+H) JetSurF 2.0 LOW / 2.66E+60 -12.00 5967.8 / ! 2*(aC3H5+H) H2/2/ CH4/2/ C2H6/3/ C4H8-2 = aC3H5+CH3 7.5E+65 -15.6 97300 ! 2012 Zhang et al. C4H8-2+H = SAXC4H7+H2 3.16E+06 2.5 6756 ! 2012 Zhang et al. C4H8-2+H=CH3CCHCH3+H2 1.32E+06 2.53 12240.0 ! EST C4H8-2+H = C3H6+CH3 3.46E+17 -1.05 6461.0 ! 2012 Zhang et al. C4H8-2+CH3 = SAXC4H7+CH4 4.40E+00 3.50 5675.0 ! Ref C3H6+CH3=aC3H5+CH3 x2 in USC Mech V2.0 C4H8-2+H = C4H7+H2 3.46E+05 2.50 2490.0 ! Ref (C3H6+H)*2 TS5 k(a) in USC Mech V2.0 C4H8-2+CH3 = C4H7+CH4 4.40E+00 3.50 5675.0 ! Ref (C3H6+CH3)*2 TS5 k(c) in USC Mech V2.0 reactions of iC4H8

iC4H7+H(+M) = iC4H8(+M) 2.00E+14 0.00 0.0 !(=(aC3H5+H) TS5 600cm-1) USC Mech V2.0 LOW / 1.33E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ CH3CCH2+CH3 (+M) = iC4H8(+M) 2.50E+13 0.00 0.0 ! Ref to C2H3+CH3 (+M) = C3H6(+M) LOW / 4.270E+58 -11.940 9769.80/ TROE / 0.175 1340.6 60000.0 10139.8 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ iC4H8+H = iC4H7+H2 1.72E+14 0.0 8000 ! 2009 Yasunaga et al. iC4H8+H = iC4H7-1+H2 1.20E+14 0.0 13000 ! 2009 Yasunaga et al. ! iC4H8+H = C3H6+CH3 8.80E+16 -1.05 6461.0 ! Ref C3H6+H = C2H4+CH3 (91TSA RRKM 0.1 atm) in USC Mech V2.0 iC4H8+CH3 = iC4H7+CH4 4.40E+00 3.50 5675.0 ! Ref C3H6+CH3=aC3H5+CH3 x2 in USC Mech V2.0 iC4H8+CH3 = iC4H7-1+CH4 2.00E+12 0.0 15000 ! 2009 Yasunaga et al.

iC4H8+H = C3H6+CH3 8.80E+16 -1.05 6461.0 !Ref USC Mech II PLOG/ 0.1 8.80E+16 -1.05 6461.0 / !Ref USC Mech II PLOG/ 1.0 8.00E+21 -2.39 11180.0 / !Ref USC Mech II PLOG/ 10 3.30E+24 -3.04 15610.0 / !Ref USC Mech II

reactions of pC4H9

pC4H9(+M) = C2H4+C2H5(+M) 1.00E+13 0.00 28366.4 ! EST LOW / 7.10E-35 15.41 -

600.0 / TROE / -5.91 333.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C4H8-1+H(+M) = pC4H9(+M) 1.33E+13 0.00 3260.7 ! =(C3H6+H) TS5 600 cm-1 USC Mech V2.0 LOW / 6.26E+38 -6.66 7000.0 / TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ pC4H9+H = C2H5+C2H5 3.40E+18 -1.33 5386.0 ! =(nC3H7+H) TS3 0.1 atm USC Mech V2.0 pC4H9+CH3 = C4H8-1+CH4 1.10E+13 0.00 0.0 ! =(nC3H7+CH3) TS3 USC Mech V2.0

reactions of sC4H9

C3H6+CH3(+M) = sC4H9(+M) 1.70E+11 0.00 7403.6 ! TS5 600cm-1 USC Mech V2.0 LOW / 2.31E+28 -4.27 1831.0 / TROE / 0.565 60000.0 534.2 3007.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C4H8-1+H(+M) = sC4H9(+M) 1.33E+13 0.00 1559.8 ! =(C3H6+H) TS5 600 cm-1 USC Mech V2.0 LOW / 8.70E+42 -7.50 4721.8 / TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C4H8-2+H(+M) = sC4H9(+M) 1.33E+13 0.00 1559.8 ! =(C3H6+H=iC3H7) TS5 600cm-1 USC Mech V2.0 LOW / 8.70E+42 -7.50 4721.8 / TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ sC4H9+H = C4H8-1+H2 3.20E+12 0.00 0.0 ! =(iC3H7+H) TS3 USC Mech V2.0 sC4H9+H = C4H8-2+H2 2.10E+12 0.00 0.0 ! =(iC3H7+H)*2/3 TS3 USC Mech V2.0 sC4H9+CH3 = CH4+C4H8-1 2.20E+14 -0.68 0.0 ! =(iC3H7+CH3) TS3 USC Mech V2.0 sC4H9+CH3 = CH4+C4H8-2 1.50E+14 -0.68 0.0 ! =(iC3H7+CH3)*2/3 TS3 USC Mech V2.0 reactions of iC4H9

C3H6+CH3(+M) = iC4H9(+M) 9.60E+10 0.00 8003.6 ! TS5 600cm-1 USC Mech V2.0 LOW / 1.30E+28 -4.27 2431.1 / TROE / 0.565 60000.0 534.2 3007.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ iC4H8+H(+M) = iC4H9(+M) 1.33E+13 0.00 3260.7 ! =(C3H6+H=nC3H7) TS5 600 cm-1 USC Mech V2.0 LOW / 6.26E+38 -6.66 7000.0 / TROE / 1.000 1000 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ iC4H9+H = iC3H7+CH3 1.10E+32 -5.04 16760.0 ! TS4 eq 0.1 atm USC Mech V2.0 iC4H9+H = iC4H8+H2 9.00E+11 0.00 0.0 ! TS4 USC Mech V2.0 iC4H9+CH3 = iC4H8+CH4 6.00E+12 -0.32 0.0 ! TS4 USC Mech V2.0 reactions of tC4H9

tC4H9(+M) = iC4H8+H(+M) 8.30E+13 0.00 38150.4 ! TS4 600cm-1 USC Mech V2.0 LOW / 1.90E+41 -7.36 36631.7/ TROE / 0.293 649.0 60000 3425.9 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ tC4H9+H = iC3H7+CH3 2.80E+34 -5.69 20500.0 ! TS4 eq 0.1 atm USC Mech V2.0 tC4H9+H = iC4H8+H2 5.42E+12 0.00 0.0 ! TS4 USC Mech V2.0 tC4H9+CH3 = iC4H8+CH4 3.80E+15 -1.00 0.0 ! TS4 USC Mech V2.0

aC3H4+C2H3 = P1XCH2C4H5-13E 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/ ! !! C2H2 + CH3CCH2 = S4XC4H4-13E2M 1.10E+31 -7.14 5600. ! Ref to C2H3 + C2H2 = nC4H5 PLOG / 0.013 1.10E+31 -7.14 5600. /

PLOG / 0.026 1.10E+32 -7.33 6200. / PLOG / 0.118 2.40E+31 -6.95 5600. / PLOG / 1.0 9.30E+38 -8.76 12000./ PLOG / 10.0 8.10E+37 -8.09 13400./ C2H3 + pC3H4 = T4XC5H7-13E 1.10E+31 -7.14 5600. ! Ref to C2H3 + C2H2 = nC4H5 PLOG / 0.013 1.10E+31 -7.14 5600. / PLOG / 0.026 1.10E+32 -7.33 6200. / PLOG / 0.118 2.40E+31 -6.95 5600. / PLOG / 1.0 9.30E+38 -8.76 12000./ PLOG / 10.0 8.10E+37 -8.09 13400./ C4H4+CH3 = S1XC4H4-13E2M 1.40E+32 -7.14 10000.0 ! Ref to C2H2+CH3 = CH3CHCH PLOG / 0.039 7.0E+31 -7.14 10000.0 / PLOG / 0.1 1.40E+32 -7.14 10000.0 / PLOG / 1.0 3.20E+35 -7.76 13300.0 / PLOG / 10.0 2.40E+38 -8.21 17100.0 / PLOG / 100.0 1.40E+39 -8.06 20200.0 / C2H2 + CH3CHCH = T1XC5H7-13E 1.10E+31 -7.14 5600. ! Ref to C2H3 + C2H2 = nC4H5 PLOG / 0.013 1.10E+31 -7.14 5600. / PLOG / 0.026 1.10E+32 -7.33 6200. / PLOG / 0.118 2.40E+31 -6.95 5600. / PLOG / 1.0 9.30E+38 -8.76 12000./ PLOG / 10.0 8.10E+37 -8.09 13400./

reactions of C5H8

C5H8-13E+H = C2H4+CH3CHCH 1.46E+30 -4.34 21647.0 ! =(C4H6+H) JetSurF 2.0 C5H8-13E+H = C4H6-2+CH3 2.00E+12 0.0 7000. ! =(C4H6+H) JetSurF 2.0 C5H8-13E+H = C4H612+CH3 2.00E+12 0.0 7000. ! =(C4H6+H) JetSurF 2.0 C5H8-13E+H = IC5H7+H2 1.73E+05 2.50 2490.0 ! (=C3H6+H) JetSurF 2.0 C5H8-13E+CH3 = IC5H7+CH4 2.20E+00 3.50 5675.0 ! =(C3H6+CH3) JetSurF 2.0 C5H8-12E = C5H8-13E 1.1E+13 0.00 67000.0 ! PLOG / 0.039 1.1E+13 0.00 67000.0 / ! /20 EST PLOG / 1.0 2.20E+14 0.00 67000.0/ ! JetSurF 2.0 C5H8-12E = C2H4+pC3H4 3.30E+11 0.00 58100.0 ! PLOG / 0.039 3.30E+11 0.00 58100.0 / ! /20 EST PLOG / 1.0 6.60E+12 0.00 58100.0/ ! JetSurF 2.0 nC4H5+CH3 = C5H8-13E 3.60E+12 0.00 0.0 ! PLOG / 0.039 3.60E+12 0.00 0.0 / ! /20 EST PLOG / 1.0 7.23E+13 0.00 0.0/ ! 04/LAU-FAR JetSurF 2.0 C5H8-14E+H = aC3H5+C2H4 1.60E+22 -2.39 11180.0 ! = C3H6+H JetSurF 2.0 C5H8-14E+H = IC5H7+H2 1.15E+05 2.50 2490.0 ! (=C3H6+H) JetSurF 2.0 C5H8-14E+H = C4H6+CH3 2.00E+12 0.0 7000. ! =(C4H6+H) JetSurF 2.0 C5H8-14E+CH3 = IC5H7+CH4 1.47E+00 3.50 5675.0 ! =(C3H6+CH3) JetSurF 2.0 C4H5-13E2M+H = C3H6+C2H3 1.46E+30 -4.34 21647.0 ! =(C4H6+H) JetSurF 2.0 C4H5-13E2M+H = CH3CCH2+C2H4 1.46E+30 -4.34 21647.0 ! =(C4H6+H) C4H5-13E2M+H = C4H6+CH3 8.00E+21 -1.39 11180.0 ! 1991 TSA RRKM 1 atm JetSurF 2.0 ori n -2.39 C4H5-13E2M+H = P1XCH2C4H5-13E+H2 1.20E+06 2.54 6760.0 ! 1989 TSA (=iC4H8+H) JetSurF 2.0 C4H5-13E2M+CH3 = P1XCH2C4H5-13E+CH4 2.20E+00 3.50 5675.0 ! =(C3H6+CH3) JetSurF 2.0 CH3+iC4H5 = C4H5-13E2M 1.00E+12 0.00 0.0 ! PLOG / 0.039 1.00E+12 0.00 0.0 / ! /20 EST PLOG / 1.0 2.00E+13 0.0 0.0/ ! JetSurF 2.0 P1XCH2C4H5-13E+H(+M) = C4H5-13E2M(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) LOW / 1.33E+60 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC5H9-1E(+M) = C4H6+CH3(+M) 3.39E+11 0.66 32262.9 ! Ref S3XC6H11-1E(+M)

= C4H6+C2H5(+M) in JetSurF 2.0 LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S3XC5H9-1E(+M) = C5H8-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ P5XC5H9-1E+H = CH3+C4H7 2.00E+21 -2.00 11000.0 ! Estimated JetSurF 2.0 P5XC5H9-1E(+M) = C2H4+aC3H5(+M) 4.57E+12 0.13 24386.4 ! Ref S5XC6H11-1E(+M) = C3H6+aC3H5(+M) LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C5H8-14E+H(+M) = P5XC5H9-1E(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S4XC5H9-1E = C5H8-13E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ C3H6+C2H3 = S4XC5H9-1E 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3=C4H7 PLOG / 0.033 6.15E+34 -7.76 9930 / PLOG / 0.1 1.23E+35 -7.76 9930 / PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/ S4XC5H9-2E(+M) = C5H8-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ P5XC5H9-2E = C5H8-13E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ CH3CHCH+C2H4 = P5XC5H9-2E 1.23E+35 -7.76 9930 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.033 6.15E+34 -7.76 9930 / PLOG / 0.1 1.23E+35 -7.76 9930 / PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/ C4H6+CH3(+M) = P4XC4H6-1E3M(+M) 9.60E+10 0.00 8003.6 ! Ref to C3H6+CH3(+M) = iC4H9(+M) LOW / 1.30E+28 -4.27 2431.1 / TROE / 0.565 60000.0 534.2 3007.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P4XC4H6-1E3M = C4H5-13E2M+H 6.35E+23 -4.75 23777 ! Ref to C4H7 = C4H6+H /2 PLOG / 0.033 6.35E+23 -4.75 23777/ PLOG / 0.066 6.90E+25 -5.221 25729/ PLOG / 0.132 8.75E+27 -5.709 27764/ PLOG / 0.197 1.58E+29 -6.003 28985/ PLOG / 0.263 1.35E+30 -6.222 29890/ PLOG / 1.0 1.24E+53 -12.30 52000/ PLOG / 10 9.25E+47 -10.50 51770/ C2H3+C3H6 = P4XC4H6-1E3M 1.23E+35 -7.76 9930 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.033 6.15E+34 -7.76 9930/ PLOG / 0.1 1.23E+35 -7.76 9930/ PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/ P4XC4H6-1E2M = C4H5-13E2M+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ CH3CCH2+C2H4 = P4XC4H6-1E2M 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.033 6.15E+34

-7.76 9930/ PLOG / 0.1 1.23E+35 -7.76 9930/ PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/

S4XC5H9-1E+H(+M) = C5H10-1E(+M) 2.40E+13 0.00 0.0 ! = iC3H7+H LOW / 1.70E+58 -12.08 11263.7 / TROE / 0.649 1213.1 1213.1 13369.7 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S3XC5H9-1E+H(+M)=C5H10-1E(+M) 2.00E+14 0.00 0.0 ! (aC3H5+H) LOW / 1.33E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P5XC5H9-1E+H(+M) = C5H10-1E(+M) 3.60E+13 0.00 0.0 ! =nC3H7+H JetSurF 2.0 LOW / 3.01E+48 -9.32 5833.6 / TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C5H10-1E=aC3H5+C2H5 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 ! PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/ C5H10-1E=C4H7+CH3 2.7E+80 -1.93E+01 1.07E+05 ! Ref to C6H12-1E=C4H7+C2H5 PLOG / 0.033 2.7E+80 -19.331 107015/ PLOG / 0.066 6.27E+68 -16.040 98670/ PLOG / 0.132 3.70E+59 -13.261 94434/ PLOG / 0.197 6.08E+61 -13.999 94475/ PLOG / 0.263 9.38E+59 -13.427 94017/ PLOG / 1.0E+5 1.46E+16 0 81020/ C5H10-1E = C3H6+C2H4 8.0E+05 1.81 53454 ! PLOG / 0.039 8.0E+05 1.81 53454/ ! 1.62E+06 /20 EST PLOG / 1 1.62E+06 1.81 53454/ ! 08/TSAwip JetSurF 2.0

C5H10-1E+H = S3XC5H9-1E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 C5H10-1E+CH3 = S3XC5H9-1E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C5H10-1E+H = S4XC5H9-1E+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 C5H10-1E+CH3 = S4XC5H9-1E+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

C5H10-1E+H = P5XC5H9-1E+H2 6.651E05 2.54 6756 ! primary LLNL-MI-407571 C5H10-1E+CH3 = P5XC5H9-1E+CH4 4.521E-1 3.65 7154 ! primary LLNL-MI-407571

SAXC4H7+CH3(+M)=C5H10-2E(+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3=C4H8-1 LOW /3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ C2H5+CH3CHCH(+M) = C5H10-2E(+M) 1.50E+13 0.00 0.0 ! Ref to C2H5+C2H3=C4H8-1 LOW /1.55E+56 -11.79 8984.5/ TROE /0.198 2277.9 60000.0 5723.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P5XC5H9-2E+H(+M) = C5H10-2E(+M) 3.60E+13 0.00 0.0 ! Ref to C4H7+H = C4H8-1 LOW / 3.01E+48 -9.32 5833.6 / TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S4XC5H9-2E+H(+M) = C5H10-2E(+M) 2.00E+14 0.00 0.0 ! Ref to SAXC4H7+H = C4H8-1 LOW / 2.66E+60 -12.00 5967.8 / H2/2/ CH4/2/ C2H6/3/ S3XC5H9-1E+H(+M) = C5H10-2E(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H = C3H6 LOW / 1.33E+60 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C5H10-2E+H = S3XC5H9-1E+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 C5H10-2E+CH3 = S3XC5H9-1E+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

C5H10-2E+H = S4XC5H9-2E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 C5H10-2E+CH3 = S4XC5H9-2E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C5H10-2E+H = P5XC5H9-2E+H2 6.651E05 2.54 6756 ! primary LLNL-MI-407571 C5H10-2E+CH3 = P5XC5H9-2E+CH4 4.521E-1 3.65 7154 ! primary LLNL-MI-407571

P1XC5H11(+M) = C2H4+nC3H7(+M) 1.00E+13 0.00 28366.4 ! 1998 TSA JetSurF 2.0 LOW / 7.10E-35 15.411 -600.0/ TROE / -5.91 333.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P1XC5H11(+M) = S2XC5H11(+M) 1.00E+12 0.00 22453.1 ! 1998 TSA JetSurF 1.1 LOW / 2.00E-26 12.833 -600.7/ TROE / -10.14 307.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C5H10-1E+H(+M) = P1XC5H11(+M) 1.33E+13 0.00 3260.7 ! Ref C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0 / TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P1XC5H11+H = nC3H7+C2H5 3.40E+18 -1.33 5386.0 ! =(nC3H7+H) 0.1 atm JetSurF 2.0 P1XC5H11+H = C5H10-1E+H2 1.80E+12 0.00 0.0 ! =(nC3H7+H) JetSurF 2.0 P1XC5H11+CH3 = C5H10-1E+CH4 1.10E+13 0.00 0.0 ! =(nC3H7+CH3) JetSurF 2.0

S2XC5H11(+M) = C3H6+C2H5(+M) 8.00E+12 0.00 27392.8 ! 1998 TSA JetSurF 2.0 LOW / 3.70E-33 14.91 -600.0 / TROE / -6.53 333.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C5H10-1E+H(+M) = S2XC5H11(+M) 1.33E+13 0.00 1559.8 ! Ref C3H6+H(+M) = iC3H7(+M) USC Mech II LOW / 8.70E+42 -7.50 4721.8/ TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S2XC5H11+H = nC3H7+C2H5 5.90E+23 -2.81 10009.0 ! =(iC3H7+H) JetSurF 2.0 S2XC5H11+H = C5H10-1E+H2 3.20E+12 0.00 0.0 ! =(iC3H7+H) JetSurF 2.0 S2XC5H11+CH3 = CH4+C5H10-1E 2.20E+14 -0.68 0.0 ! =(iC3H7+CH3) JetSurF 2.0 S3XC5H11(+M) = C4H8-1+CH3(+M) 1.80E+13 0.00 29348.0 ! 1998 TSA JetSurF 2.0 LOW / 4.00E-39 16.782 -600.4/ TROE / -7.03 314.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

IC5H7(+M)+CH3 = C6H10-13E(+M) 1.00E+14 -0.32 -262.3 ! 1991 TSA JetSurF 2.0 LOW / 3.91E+60 -12.81 6250.0 / TROE / 0.104 1606.0 60000.0 6118.4 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C6H10-13E+H = C4H8-1+C2H3 1.46E+30 -4.34 21647.0 ! =(C4H6+H) JetSurF 2.0

C6H10-13E + H = S5XC6H9-13E + H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 C6H10-13E + CH3 = S5XC6H9-13E + CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H10-15E = aC3H5+aC3H5 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132

1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H10-15E + H = S3XC6H9-15E + H2 6.752E05 2.36 207 ! (ax4) allyls LLNL-MI-407571 C6H10-15E + CH3 = S3XC6H9-15E + CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571

S5XC6H9-13E(+M) = C6H8-135E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7 LOW / 4.6E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S3XC6H9-15E = C6H8-135E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ C4H6+C2H3 = S3XC6H9-15E 1.23E+35 -7.76 9930 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930/ PLOG / 0.1 1.23E+35 -7.76 9930/ PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/

C2H3 + nC4H5 = C6H8-135E 7.00E+57 -13.82 17629. ! Ref to C2H3+C2H3=C4H6 PLOG / 0.026 7.00E+57 -13.82 17629/ PLOG / 0.118 1.50E+52 -11.97 16056/ PLOG / 1.0 1.50E+42 -8.84 12483/

P6XC6H9-13E = C6H8-135E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ C2H4+nC4H5=P6XC6H9-13E 1.23E+35 -7.76 9930 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930/ PLOG / 0.1 1.23E+35 -7.76 9930/ PLOG / 1.0 7.93E+38 -8.47 14220/ PLOG / 10 2.99E+36 -7.40 15480/

C6H8-135E+H = C2H4+nC4H5 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H8-135E+H = C2H3+C4H6 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3

!cC6H10 cC6H9 cC6H8 reactions

cC6H10 = C4H6+C2H4 5.0E+78 -18.94 98386 ! EST PLOG / 0.039 5.0E+78 -18.94 98386/ PLOG / 0.197 2.60E+70 -16.36 95510/ PLOG / 1.0 3.81E+25 -3.58 64034/ PLOG / 1.0E+5 8.31E+13 0.387 64116/

S2XcC6H9-1E+H(+M) = cC6H10(+M) 2.66E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *4/3 LOW / 1.77E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

cC6H10+H = S2XcC6H9-1E+H2 6.752E05 2.36 207 ! (ax4) allyls LLNL-MI-407571 cC6H10 + CH3 = S2XcC6H9-1E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571

cC6H10+H=S3XcC6H9-1E+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 cC6H10+CH3=S3XcC6H9-1E+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

S2XcC6H9-1E = cC6H8-13E+H 2.67E+12 0.71 49792.2 ! JetSurF 2.0 PLOG / 0.039 1.62E+57 -13.03 66036/ ! 2011 Li et al. PLOG / 1.0 2.67E+12 0.71 49792.2/ ! JetSurF 2.0 S2XcC6H9-1E=P6XC6H9-13E 1.30E+13 0.00 35900 ! 2003 Dayma et al. PLOG / 0.039 5.36E+50 -11.92 48276/ ! 2011 Li et al. PLOG / 1.0 1.30E+13 0.00 35900/ ! 2003 Dayma et al.

S2XcC6H9-1E+H = cC6H8-13E+H2 1.80E+13 0.00 0.0 ! Ref to SAXC4H7+H

S3XcC6H9-1E=S3XC6H9-15E 1.1E12 0.53 16166 ! Gong 2012 S3XcC6H9-1E = cC6H8-14E+H 2.14E+11 0.92 46792 ! Gong 2012, Refer to S3XcC6H9-1E = cC6H8-13E+H S3XcC6H9-1E = cC6H8-13E+H 9.12E9 0.88 34639 ! Gong 2012, P6XC6H9-13E = C6H8-135E+H

cC6H8-13E+H = S1XcC6H7-24E+H2 6.752E05 2.36 207 ! (ax4) allyls LLNL-MI-407571 cC6H8-13E + CH3 = S1XcC6H7-24E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571

S1XcC6H7-24E=A1+H 6.76E+11 0.78 30230 ! PLOG / 0.039 3.40E+10 0.78 30230/ ! /20 EST PLOG / 1.0 6.76E+11 0.78 30230/ ! JetSurF 2.0 S1XcC6H7-24E+H = A1+H2 1.80E+13 0.00 0.0 ! Ref to SAXC4H7+H

! C6H11 reactions

P6XC6H11-1E(+M) = C4H7+C2H4(+M) 3.98E+12 0.12 27571.6 ! JetSurF 2.0 LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C6H10-15E+H(+M) = P6XC6H11-1E(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ P6XC6H11-1E(+M) = S3XC6H11-1E(+M) 1.55E+02 2.83 15566.2 ! JetSurF 2.0 LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S3XC6H11-1E(+M) = C4H6+C2H5(+M) 3.39E+11 0.66 32262.9 ! JetSurF 2.0 LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S3XC6H11-1E(+M) = C6H10-13E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S3XC6H11-1E+H=C6H10-13E+H2 1.60E+12 0.00 0.0 ! Ref to iC3H7+H /2 S3XC6H11-1E+CH3=C6H10-13E+CH4 4.7E+10 0.68 0.0 ! Ref to iC3H7+CH3 /2

S5XC6H11-1E(+M) = C3H6+aC3H5(+M) 4.57E+12 0.13 24386.4 ! JetSurF 2.0 LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C6H10-15E+H(+M) = S5XC6H11-1E(+M) 1.33E+13 0.00 1559.8 ! Ref to C4H8-1+H(+M) = sC4H9(+M) LOW / 8.70E+42 -7.50 4721.8 / TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC6H11-1E(+M) = C5H8-14E+CH3(+M) 8.13E+10 0.78 29648.0 ! 2007 TSA JetSurF 2.0 LOW / 4.00E-39 16.782 -600.4 / TROE / -7.03 314.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S4XC6H11-1E = C6H10-13E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/

S4XC6H11-1E+H = nC3H7+aC3H5 2.00E+21 -2.00 11000 ! Ref to C4H7+H S4XC6H11-1E+H = C6H10-13E+H2 1.80E+12 0.00 0.0 ! Ref to C4H7+H S4XC6H11-1E+CH3 = C6H10-13E+CH4 1.10E+13 0.00 0.0 ! Ref to C4H7+CH3

P1XCH2cC5H9=P6XC6H11-1E 8.92E+18 -2.94 19897 ! Ref to PXCH2cC6H11=P7XC7H13-1E PLOG / 0.039 8.92E+18 -2.94 19897 / PLOG / 0.197 6.83E+22 -3.82 23511 / PLOG / 1.000 1.56E+29 -5.39 29211 / PLOG / 10.000 4.15E+37 -7.44 37753 / PLOG / 100.000 1.92E+39 -7.58 42286 / PLOG / 1.0E+5 2.53E+13 0.16 29785 /

P1XCH2cC5H9=CH2cC5H8+H 8.14E+14 -2.42 21719 ! Ref to PXCH2cC6H11=CH2cC6H10+H PLOG / 0.039 8.14E+14 -2.42 21719 / PLOG / 0.197 1.23E+20 -3.61 26095 / PLOG / 1.000 1.18E+28 -5.58 32946 / PLOG / 10.000 1.31E+39 -8.28 43693 / PLOG / 100.000 4.67E+42 -8.87 50298 / PLOG / 1.0E+5 1.60E+11 0.59 35447 /

P1XCH2cC5H9(+M) = S3XcC5H81M(+M) 6.61E+01 2.85 21082.1 ! 08/TSAwip JetSurF 2.0 LOW / 1.10E-36 16.12 -602.5 / TROE / -21.57 225 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XcC5H81M=P5XC5H8-1E4M 1.21E+18 -2.84 19903 ! Ref to S3XMCH=P6XC6H10-1E4M PLOG / 0.039 1.21E+18 -2.84 19903 / PLOG / 0.197 7.98E+21 -3.70 23365 / PLOG / 1.000 2.52E+28 -5.31 28978 / PLOG / 10.000 8.05E+37 -7.66 38033 / PLOG / 100.000 6.13E+42 -8.70 44718 / PLOG / 1.0E+5 1.68E+13 0.21 31241 /

S3XcC5H81M=S5XC6H11-1E 5.23E+18 -2.93 19555 ! Ref to S3XMCH=S6XC7H13-1E PLOG / 0.039 5.23E+18 -2.93 19555 / PLOG / 0.197 2.06E+22 -3.73 22876 / PLOG / 1.000 3.29E+28 -5.27 28275 / PLOG / 10.000 3.31E+37 -7.49 36918 / PLOG / 100.000 8.80E+41 -8.42 43157 / PLOG / 1.0E+5 2.55E+13 0.17 30061 /

P5XC5H8-1E4M(+M) = aC3H5+C3H6(+M) 5.37E+12 0.12 23947.3 ! 08/TSAwip JetSurF 2.0 LOW / 4.90E-31 14.54 -578.8 / TROE / -11.90 267 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!cC6H11 reactions

cC6H11=P6XC6H11-1E 1.26E+22 -3.85 22627 ! Ref to S4XMCH=P6XC6H10-1E5M PLOG / 0.039 1.26E+22 -3.85 22627 / PLOG / 0.197 3.57E+26 -4.89 26638 / PLOG / 1.000 2.59E+32 -6.32 32020 / PLOG / 10.000 2.07E+41 -8.51 40814 / PLOG / 100.000 5.79E+44 -9.15 46530 / PLOG / 1.0E+5 3.87E+13 0.20 31782 /

cC6H11=cC6H10+H 8.38E+20 -3.63 23771 ! Ref to S4XMCH=MCH-3E+H PLOG / 0.039 8.38E+20 -3.63 23771 / PLOG / 0.197 8.32E+25 -4.80 28120 / PLOG / 1.000 5.73E+32 -6.47 34206 / PLOG / 10.000 1.37E+43 -9.02 44242 / PLOG / 100.000 7.21E+47 -9.98 51272 / PLOG / 1.0E+5 3.78E+12 0.63 34881 /

cC6H11+H = cC6H10+H2 3.60E+12 0.00 0.0 ! Ref to nC3H7+H *2 cC6H11+CH3 = cC6H10+CH4 2.20E+13 -0.32 0.0 ! Ref to nC3H7+CH3 *2

!C6H12-1E reactions

P6XC6H11-1E+H(+M) = C6H12-1E(+M) 3.60E+13 0.00 0.0 ! = nC3H7+H LOW / 3.01E+48 -9.32 5833.6 / TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S5XC6H11-1E+H(+M) = C6H12-1E(+M) 2.40E+13 0.00 0.0 ! = iC3H7+H LOW / 1.70E+58 -12.08 11263.7/ TROE / 0.649 1213.1 1213.1 13369.7 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S4XC6H11-1E+H(+M) = C6H12-1E(+M) 2.40E+13 0.00 0.0 ! = iC3H7+H LOW / 1.70E+58 -12.08 11263.7/ TROE / 0.649 1213.1 1213.1 13369.7 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ S3XC6H11-1E+H(+M)=C6H12-1E(+M) 2.00E+14 0.00 0.0 ! = (aC3H5+H) LOW / 1.33E+60 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ C6H12-1E=aC3H5+nC3H7 1.07E+80 -19.33 95177 ! PLOG / 0.039 1.07E+80 -19.33 95177/ ! 2009 Kiefer et al. PLOG / 0.066 2.50E+68 -16.040 86832/ ! 2009 Kiefer et al. PLOG / 0.132 1.480E+59 -13.261 82596/ ! 2009 Kiefer et al. PLOG / 0.197 2.43E+61 -13.999 82637/ ! 2009 Kiefer et al. PLOG / 0.263 3.75E+59 -13.427 82179/ ! 2009 Kiefer et al. PLOG / 1.0E+5 1.46E+16 0.00 69120/ ! 2009 Kiefer et al. C6H12-1E=C4H7+C2H5 2.7E+80 -19.331 107015 PLOG / 0.033 2.7E+80 -19.331 107015/ ! 2009 Kiefer et al. PLOG / 0.066 6.27E+68 -16.040 98670/ ! 2009 Kiefer et al. PLOG / 0.132 3.70E+59 -13.261 94434/ ! 2009 Kiefer et al. PLOG / 0.197 6.08E+61 -13.999 94475/ ! 2009 Kiefer et al. PLOG / 0.263 9.38E+59 -13.427 94017/ ! 2009 Kiefer et al. PLOG / 1.0E+5 1.46E+16 0.0 81020/ ! EST C6H12-1E = C3H6+C3H6 7.08E+06 1.65 53752.0 ! PLOG / 0.039 3.54E+05 1.65 53752.0 / ! /20 EST PLOG / 1.0 7.08E+06 1.65 53752.0 / ! JetSurF 2.0

C6H12-1E+H=S3XC6H11-1E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 C6H12-1E+CH3=S3XC6H11-1E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H12-1E+H=S5XC6H11-1E+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 C6H12-1E+CH3=S5XC6H11-1E+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

C6H12-1E+H=S4XC6H11-1E+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 C6H12-1E+CH3=S4XC6H11-1E+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

C6H12-1E+H = P6XC6H11-1E+H2 6.651E05 2.54 6756 ! primary LLNL-MI-407571 C6H12-1E+CH3 = P6XC6H11-1E+CH4 4.521E-1 3.65 7154 ! primary LLNL-MI-407571

cC6H12 reactions

cC6H11+H(+M)=cC6H12(+M) 4.80E+13 0.00 0.0 ! =(iC3H7+H) JetSurF 2.0 LOW / 1.70E+58 -12.08 11263.7/ TROE / 0.649 1213.1 1213.1 13369.7 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ cC6H12=C6H12-1E 1.33E+137 -34.70 162775 ! 2009 Kiefer et al. PLOG / 0.039 1.33E+137 -34.70 162775/ ! /1.5 PLOG / 0.066 5.96E+139 -35.26 166598/ ! PLOG / 0.263 1.82E+143 -35.99 172904/ ! PLOG / 1.0E+5 8.76E+17 0.00 91940 / ! cC6H12+H=cC6H11+H2 2.70E+10 1.385 8229 ! 2009 Kiefer et al. cC6H12+CH3=cC6H11+CH4 9.06E+00 3.46 5480 ! Ref to C3H8+CH3=iC3H7+CH4 *6

A1CH2+H(+M)=CH2cC6H6-13E(+M) 4.98E11 0.611 -436 ! oit 2007 Klippenstein LOW / 1.34E52 -10.3 -3910 / TROE / 0.01 1 -1300 50000/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/ A1CH2+H(+M)=CH2cC6H6-25E(+M) 6.44E12 0.245 -333 ! pit 2007 Klippenstein LOW / 2.62E45 -8.59 -11590/ TROE / 0.025 1 -5000 50000/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2cC6H6-13E+H=A1CH2+H2 6.47E00 3.98 3394.0 ! Ref to A1CH3 CH2cC6H6-13E+CH3=A1CH2+CH4 3.160E+11 0.000 9500.00 ! Ref to A1CH3

CH2cC6H6-25E+H=A1CH2+H2 6.47E00 3.98 3394.0 ! Ref to A1CH3 CH2cC6H6-25E+CH3=A1CH2+CH4 3.160E+11 0.000 9500.00 ! Ref to A1CH3

!cC7H9 reactions

S5XMCH-13E(+M)=A1CH3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE /-51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S6XMCH-13E(+M)=A1CH3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ S3XMCH-15E(+M)=A1CH3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M)

= C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ S4XMCH-15E(+M)=A1CH3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ S2XMCH-35E(+M)=A1CH3+H(+M) 1.56E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *1/3 LOW / 1.53E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S2XMCH-35E=A1+CH3 4.24E+21 -3.89 22867 ! Ref to S2XMCH=cC6H10+CH3 PLOG / 0.039 4.24E+21 -3.89 22867 / ! PLOG / 0.197 2.58E+22 -3.86 24360 / ! PLOG / 1.000 2.27E+28 -5.30 29571 / ! PLOG / 10.000 4.14E+38 -7.84 39088 / ! PLOG / 100.000 1.94E+45 -9.36 47105 / ! PLOG / 1.0E+5 6.35E+13 0.20 33524 / !

T1XMCH-35E(+M)=A1CH3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

!T1XMCH-35E(+M)=CH2cC6H6-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) ! 20131224 shielded ! LOW / 4.6E-37 15.37 -603.1 / ! TROE / -51.87 258 28 50000.0 / ! H2/2/ CH4/2/ C2H6/3/

CH2S4XcC6H7-5E(+M)=CH2cC6H6-13E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ CH2S2XcC6H7-5E(+M)=CH2cC6H6-25E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

! cC7H10 reactions

MCH-13E+H = S5XMCH-13E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-13E+CH3= S5XMCH-13E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S5XMCH-13E+H(+M)=MCH-13E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M *2/3 LOW /0.89E+60 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S6XMCH-13E+H(+M)=MCH-13E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M *2/3 LOW /0.89E+60 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-13E+H = S6XMCH-13E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-13E+CH3= S6XMCH-13E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

MCH-13E+H = CH2S4XcC6H7-5E+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 MCH-13E+CH3= CH2S4XcC6H7-5E+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

CH2S4XcC6H7-5E+H(+M)=MCH-13E(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) LOW /1.33E+60 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-15E+H = S3XMCH-15E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-15E+CH3= S3XMCH-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S3XMCH-15E+H(+M)=MCH-15E(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW /0.89E+59 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-15E+H = S4XMCH-15E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-15E+CH3= S4XMCH-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S4XMCH-15E+H(+M)=MCH-15E(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW /0.89E+59 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-15E+H = CH2S2XcC6H7-5E+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 MCH-15E+CH3= CH2S2XcC6H7-5E+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

CH2S2XcC6H7-5E+H(+M)=MCH-15E(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) LOW /1.33E+60 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/ ! MCH-35E+H = S2XMCH-35E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-35E+CH3= S2XMCH-35E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S2XMCH-35E+H(+M)=MCH-35E(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-35E+H = T1XMCH-35E+H2 2.65E6 2.2 0.0 ! allylt LLNL-MI-407571 MCH-35E+CH3= T1XMCH-35E+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

T1XMCH-35E+H(+M)=MCH-35E(+M) 0.67E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *1/3 LOW / 0.44E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S1XcC6H7-24E+CH3(+M)=MCH-35E(+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4H8-1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

CH2cC6H8-2E+H = CH2S4XcC6H7-5E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 CH2cC6H8-2E+CH3= CH2S4XcC6H7-5E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2S4XcC6H7-5E+H(+M)=CH2cC6H8-2E(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2cC6H8-2E+H = CH2S2XcC6H7-5E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 CH2cC6H8-2E+CH3= CH2S2XcC6H7-5E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2S2XcC6H7-5E+H(+M)=CH2cC6H8-2E(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! C6H7-135E2M,C6H7-135E3M, C7H10-135E reactions

C6H7-135E2M+H = C4H6+CH3CCH2 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E2M+H = S4XC4H4-13E2M+C2H4 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E2M+H = C6H8-135E+CH3 8.80E+16 -1.05 6461.0 ! Ref to C3H6+H = C2H4+CH3 C6H7-135E2M+H = C3H6+nC4H5 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E2M+H = C4H5-13E2M+C2H3 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3

C6H7-135E3M+H = T4XC5H7-13E+C2H4 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E3M+H = S1XC4H4-13E2M+C2H4 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E3M+H = C4H5-13E2M+C2H3 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E3M+H = C5H8-13E+C2H3 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C6H7-135E3M+H = C6H8-135E+CH3 8.80E+16 -1.05 6461.0 ! Ref to C3H6+H = C2H4+CH3

C7H10-135E+H = T1XC5H7-13E+C2H4 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C7H10-135E+H = C4H6+CH3CHCH 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C7H10-135E+H = C6H8-135E+CH3 8.80E+16 -1.05 6461.0 ! Ref to C3H6+H = C2H4+CH3 C7H10-135E+H = C5H8-13E+C2H3 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3 C7H10-135E+H = nC4H5+C3H6 1.46E+30 -4.34 21647 ! Ref to C4H6+H = C2H4+C2H3

!cyclic C7H11 reactions

S3XMCH-1E(+M)=MCH-13E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE /-51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ S2XMCH-6E(+M)=MCH-15E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ T1XMCH-2E(+M)=MCH-15E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ T1XMCH-2E(+M)=CH2cC6H8-2E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW / 4.60E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S2XMCH-3E(+M)=MCH-35E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE /-51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ S2XMCH-3E(+M)=MCH-13E+H(+M) 1.57E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *1/3 LOW/ 1.54E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S2XMCH-3E=cC6H8-13E+CH3 4.24E+21 -3.89 22867 ! Ref to S2XMCH=cC6H10+CH3 PLOG / 0.039 4.24E+21 -3.89 22867 / ! PLOG / 0.197 2.58E+22 -3.86 24360 / ! PLOG / 1.000 2.27E+28 -5.30 29571 / ! PLOG / 10.000 4.14E+38 -7.84 39088 / ! PLOG / 100.000 1.94E+45 -9.36 47105 / ! PLOG / 1.0E+5 6.35E+13 0.20 33524 / !

S5XMCH-3E(+M)=MCH-35E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S3XC7H11-16E(+M) = C4H6+aC3H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC7H11-15E = C7H10-135E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/ C4H6+CH3CHCH =S3XC7H11-15E 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

S4XC7H11-15E = C7H10-135E+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777 / PLOG / 0.066 1.38E+26 -5.221 25729 / PLOG / 0.132 1.75E+28

-5.709 27764 / PLOG / 0.197 3.16E+29 -6.003 28985 / PLOG / 0.263 2.69E+30 -6.222 29890 / PLOG / 1.0 2.48E+53 -12.30 52000 / PLOG / 10 1.85E+48 -10.50 51770 / C5H8-13E+C2H3 = S4XC7H11-15E 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

S7XC7H11-15E(+M) = C4H6+aC3H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

T3XC6H8-15E3M = C6H7-135E3M+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777 / PLOG / 0.066 1.38E+26 -5.221 25729 / PLOG / 0.132 1.75E+28 -5.709 27764 / PLOG / 0.197 3.16E+29 -6.003 28985 / PLOG / 0.263 2.69E+30 -6.222 29890 / PLOG / 1.0 2.48E+53 -12.30 52000 / PLOG / 10 1.85E+48 -10.50 51770 / C4H5-13E2M+C2H3 = T3XC6H8-15E3M 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

S4XC6H8-15E3M (+M) = C6H8-135E+CH3 (+M) 3.39E+11 0.66 32262.9 ! Ref S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C5H8-13E+C2H3 = S4XC6H8-15E3M 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

S4XC6H8-15E3M(+M) = C6H7-135E3M+H(+M) 1.57E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *1/3 LOW/ 1.54E-37 15.37 -603.1 / TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

P1XCH2-3C6H9-15E(+M) = C4H6+aC3H5(+M) 4.57E+12 0.13 24386.4 ! Ref to S5XC6H11-1E(+M) = C3H6+aC3H5(+M) LOW / 2.50E-31 14.57 -578.8/ TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H8-15E2M = C6H7-135E2M+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777 / PLOG / 0.066 1.38E+26 -5.221 25729 / PLOG / 0.132 1.75E+28 -5.709 27764 / PLOG / 0.197 3.16E+29 -6.003 28985 / PLOG / 0.263 2.69E+30 -6.222 29890 / PLOG / 1.0 2.48E+53 -12.30 52000 / PLOG / 10 1.85E+48 -10.50 51770 / C4H5-13E2M+C2H3 = S3XC6H8-15E2M 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34

-7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

S4XC6H8-15E2M = C6H7-135E2M+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777 / PLOG / 0.066 1.38E+26 -5.221 25729 / PLOG / 0.132 1.75E+28 -5.709 27764 / PLOG / 0.197 3.16E+29 -6.003 28985 / PLOG / 0.263 2.69E+30 -6.222 29890 / PLOG / 1.0 2.48E+53 -12.30 52000 / PLOG / 10 1.85E+48 -10.50 51770 / C4H6+CH3CCH2 = S4XC6H8-15E2M 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

P1XCH2C6H9-15E=aC3H4+C4H7 1.00E+12 0.0 51000 ! Ref to iC4H7=aC3H4+CH3 PLOG / 0.039 1.00E+12 0.0 51000/ ! EST /10 PLOG / 1.0 1.00E+13 0.0 51000/ ! 2009 Yasunaga et al.

!cC7H12 reactions

MCH-1E+H = S3XMCH-1E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-1E+CH3= S3XMCH-1E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S3XMCH-1E+H(+M)=MCH-1E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.89E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S2XMCH-6E+H(+M)=MCH-1E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.89E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-1E+H = S2XMCH-6E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-1E+CH3= S2XMCH-6E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2S2XcC6H9+H(+M)=MCH-1E(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) LOW /1.33E+60 -12.00 5967.8/ TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-1E+H = CH2S2XcC6H9+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 MCH-1E+CH3= CH2S2XcC6H9+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

MCH-2E+H = S2XMCH-3E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-2E+CH3= S2XMCH-3E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S2XMCH-3E+H(+M)=MCH-2E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.89E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-2E+H = T1XMCH-2E+H2 2.65E6 2.2 0.0 ! allylt LLNL-MI-407571 MCH-2E+CH3= T1XMCH-2E+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

T1XMCH-2E+H(+M)=MCH-2E(+M) 0.67E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *1/3 LOW / 0.44E+60 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S2XcC6H9-1E+CH3(+M)=MCH-2E(+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4H8-1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

MCH-3E+H = S2XMCH-3E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-3E+CH3= S2XMCH-3E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S2XMCH-3E+H(+M)=MCH-3E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

MCH-3E+H = S5XMCH-3E+H2 3.376E05 2.36 207 ! allyls LLNL-MI-407571 MCH-3E+CH3= S5XMCH-3E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

S5XMCH-3E+H(+M)=MCH-3E(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+60 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2cC6H10+H = CH2S2XcC6H9+H2 6.752E05 2.36 207 ! (ax4) allyls LLNL-MI-407571 CH2cC6H10+CH3= CH2S2XcC6H9+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571

CH2S2XcC6H9+H(+M)=CH2cC6H10(+M) 4.0E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2 LOW / 2.66E+60 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2S2XcC6H9=C2H3-2-PXC5H8 1.24E+22 -4.01 22066 ! Ref to S2XMCH=P6XC6H10-1E3M ! 20131221 added PLOG / 0.039 1.24E+22 -4.01 22066 / ! PLOG / 0.197 4.17E+22 -3.93 23430 / ! PLOG / 1.000 1.01E+28 -5.23 28271 / ! PLOG / 10.000 2.14E+37 -7.54 37062 / ! PLOG / 100.000 1.11E+43 -8.81 44209 / ! PLOG / 1.0E+5 1.59E+13 0.22 31118 / !

CH2S2XcC6H9=CH2cC6H8-2E+H 1.82E+20 -3.68 23447 ! Ref to S2XMCH=MCH-2E+H ! 20131221 added PLOG / 0.039 1.82E+20 -3.68 23447 / ! PLOG / 0.197 1.92E+21 -3.70 25053 / ! PLOG / 1.000 5.62E+27 -5.27 30610 / ! PLOG / 10.000 7.34E+38 -8.02 40816 / ! PLOG / 100.000 2.67E+46 -9.75 49698 / ! PLOG / 1.0E+5 2.01E+12 0.63 35196 / !

CH2cC6H10+H = CH2S3XcC6H9+H2 2.6E+06 2.4 4471 ! secondary LLNL-MI-407571 ! 20131221 added 1.3E06 *2 CH2cC6H10+CH3 = CH2S3XcC6H9+CH4 3.0E+00 3.46 5481 ! secondary LLNL-MI-407571 ! 20131221 added 1.51 *2

CH2S3XcC6H9=CH2-4-PXC6H9 1.21E+18 -2.84 19903 ! Ref to S3XMCH=P6XC6H10-1E4M ! 20131221 added PLOG / 0.039 1.21E+18 -2.84 19903 / ! PLOG / 0.197 7.98E+21 -3.70 23365 / ! PLOG / 1.000 2.52E+28 -5.31 28978 / ! PLOG / 10.000 8.05E+37 -7.66 38033 / ! PLOG / 100.000 6.13E+42 -8.70 44718 / ! PLOG / 1.0E+5 1.68E+13 0.21 31241 / !

CH2S3XcC6H9=CH2cC6H8-2E+H 1.27E+24 -4.75 23777 ! Ref to C4H7=C4H6+H ! 20131221 added PLOG / 0.033 1.27E+24 -4.75 23777 / ! PLOG / 0.066 1.38E+26 -5.221 25729 / ! PLOG / 0.132 1.75E+28 -5.709 27764 / ! PLOG / 0.197 3.16E+29 -6.003 28985 / ! PLOG / 0.263 2.69E+30 -6.222 29890 / ! PLOG / 1.0 2.48E+53 -12.30 52000 / ! PLOG / 10 1.85E+48 -10.50 51770 / !

CH2-4-PXC6H9=CH2-3-C6H8-14+H 1.27E+24 -4.75 23777 ! Ref to C4H7=C4H6+H ! 20131221 added PLOG / 0.033 1.27E+24 -4.75 23777 / ! PLOG / 0.066 1.38E+26 -5.221 25729 / ! PLOG / 0.132 1.75E+28 -5.709 27764 / ! PLOG / 0.197 3.16E+29 -6.003 28985 / ! PLOG / 0.263 2.69E+30 -6.222 29890 / ! PLOG / 1.0 2.48E+53 -12.30 52000 / ! PLOG / 10 1.85E+48 -10.50 51770 / !

CH2-3-C6H8-14+H = P1XCH2C4H5-13E+C2H4 8.80E+16 -1.05 6461.0 ! Ref C3H6+H = C2H4+CH3 ! 20131221 added CH2-3-C6H8-14+H = C4H6+aC3H5 8.80E+16 -1.05 6461.0 ! Ref C3H6+H = C2H4+CH3 ! 20131221 added

CH2cC6H10+H = CH2S4XcC6H9+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 ! 20131221 added CH2cC6H10+CH3 = CH2S4XcC6H9+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571 ! 20131221 added

CH2S4XcC6H9=CH2-5-PXC6H9 1.26E+22 -3.85 22627 ! Ref to S4XMCH PLOG / 0.039 1.26E+22 -3.85 22627 / ! PLOG / 0.197 3.57E+26 -4.89 26638 / ! PLOG / 1.000 2.59E+32 -6.32 32020 / ! PLOG / 10.000 2.07E+41 -8.51 40814 / ! PLOG / 100.000 5.79E+44 -9.15 46530 / ! PLOG / 1.0E+5 3.87E+13 0.20 31782 / !

CH2-5-PXC6H9=aC3H4+C4H7 7.010E+10 1.38 56000 ! Ref to iC4H7=aC3H4+CH3, hpl,2005ZHE/SUN9044-9053 J. Phys. Chem. A 109

MCH-1E=C4H5-13E2M+C2H4 5.0E+78 -18.94 98386 ! Ref to cC6H10 = C4H6+C2H4 PLOG / 0.039 5.0E+78 -18.94 98386 / PLOG / 0.197 2.60E+70 -16.36 95510 / PLOG / 1.0 3.81E+25 -3.58 64034 / PLOG / 1.0E+5 8.31E+13 0.387 64116 /

MCH-2E=C5H8-13E+C2H4 5.0E+78 -18.94 98386 ! Ref to cC6H10 = C4H6+C2H4 PLOG / 0.039 5.0E+78 -18.94 98386 / PLOG / 0.197 2.60E+70 -16.36 95510 / PLOG / 1.0 3.81E+25 -3.58 64034 / PLOG / 1.0E+5 8.31E+13 0.387 64116 /

MCH-3E=C4H6+C3H6 5.0E+78 -18.94 98386 ! Ref to cC6H10 = C4H6+C2H4 PLOG / 0.039 5.0E+78 -18.94 98386 / PLOG / 0.197 2.60E+70 -16.36 95510 / PLOG / 1.0 3.81E+25 -3.58 64034 / PLOG / 1.0E+5 8.31E+13 0.387 64116 /

CH2cC6H10=C6H9-15E2M 1.33E+137 -34.70 162775 ! Ref to cC6H12 PLOG / 0.039 1.33E+137 -34.70 162775/ ! PLOG / 0.066 5.96E+139 -35.26 166598/ ! PLOG / 0.263 1.82E+143 -35.99 172904/ ! PLOG / 1.0E+5 8.76E+17 0.00 91940 / !

! C7H12 dienes reactions

C7H12-13E+H = C5H10-1E+C2H3 1.46E+30 -4.34 21647.0 ! =(C4H6+H) C7H12-13E= C2H5+IC5H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C7H12-16E=aC3H5+C4H7 2.14E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 *2 PLOG / 0.039 2.14E+80 -19.33 95177/ PLOG / 0.066 5.00E+68 -16.040 86832/ PLOG / 0.132 2.96E+59 -13.261 82596/ PLOG / 0.197 4.86E+61 -13.999 82637/ PLOG / 0.263 7.50E+59 -13.427 82179/ PLOG / 1.0E+5 2.92E+16 0.00 69120/

C7H12-16E+H = S3XC7H11-16E+H2 6.752E+5 2.36 207 ! (ax4) allyls LLNL-MI-407571 C7H12-16E+CH3 = S3XC7H11-16E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571 C7H12-16E+H = T2XC7H11-16E+H2 6.752E+5 2.36 207 ! (ax4) allyls LLNL-MI-407571 C7H12-16E+CH3 = T2XC7H11-16E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571 C7H12-16E+H = T1XC7H11-16E+H2 6.752E+5 2.36 207 ! (ax4) allyls LLNL-MI-407571 C7H12-16E+CH3 = T1XC7H11-16E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571 !C7H12-16E+H = S4XC7H11-16E+H2 6.752E+5 2.36 207 ! (ax4) allyls LLNL-MI-407571 !C7H12-16E+CH3 = S4XC7H11-16E+CH4 7.38 3.31 4002 ! (ax4) allyls LLNL-MI-407571

C7H12-15E= aC3H5+SAXC4H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C7H12-15E+H =S3XC7H11-15E+H2 3.376E5 2.36 207 ! allyls LLNL-MI-407571 C7H12-15E+H = S4XC7H11-15E+H2 3.376E5 2.36 207 ! allyls LLNL-MI-407571 C7H12-15E+CH3 =S3XC7H11-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571 C7H12-15E+CH3 = S4XC7H11-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C7H12-15E+H = S7XC7H11-15E+H2 1.7298E5 2.5 2492 ! allylP LLNL-MI-407571 C7H12-15E+CH3 = S7XC7H11-15E+CH4 2.2098 3.5 5675 ! allylP LLNL-MI-407571

C6H9-15E3M = aC3H5+SAXC4H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H9-15E3M = S3XC6H9-15E+CH3 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H9-15E3M+H = S4XC6H8-15E3M+H2 3.376E5 2.36 207 ! allyls LLNL-MI-407571 C6H9-15E3M+CH3 = S4XC6H8-15E3M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H9-15E3M+H = P1XCH2-3C6H9-15E+H2 6.651E05 2.54 6756 ! primary LLNL-MI-407571 C6H9-15E3M+CH3 = P1XCH2-3C6H9-15E+CH4 4.521E-1 3.65 7154 ! primary LLNL-MI-407571

C6H9-15E3M+H = T3XC6H8-15E3M+H2 2.65E6 2.2 0.0 ! allylt LLNL-MI-407571 C6H9-15E3M+CH3 = T3XC6H8-15E3M+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

C7H12-24E = S5XC6H9-13E+CH3 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

CH2-3-C6H10-1E = P1XCH2C4H5-13E+C2H5 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

CH2-3-C6H10-1E+H = C5H10-1E+C2H3 1.46E+30 -4.34 21647.0 ! =(C4H6+H) CH2-3-C6H10-1E+H = C4H6+nC3H7 8.80E+16 -1.05 6461.0 ! Ref to C3H6+H = C2H4+CH3 CH2-3-C6H10-1E+H = C4H5-13E2M+C2H5 3.20E+22 -2.39 11180 ! Ref to C4H8-1+H = C3H6+CH3 C6H9-15E2M+H = S3XC6H8-15E2M+H2 3.376E5 2.36 207 ! allyls LLNL-MI-407571 C6H9-15E2M+H = S4XC6H8-15E2M+H2 3.376E5 2.36 207 ! allyls LLNL-MI-407571

C6H9-15E2M+H = P1XCH2C6H9-15E+H2 1.7298E5 2.5 2492 ! allylp LLNL-MI-407571 C6H9-15E2M+CH3 = S3XC6H8-15E2M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571 C6H9-15E2M+CH3 = S4XC6H8-15E2M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H9-15E2M+CH3 = P1XCH2C6H9-15E+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

C6H9-15E2M = aC3H5+iC4H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H9-13E5M = S5XC6H9-13E+CH3 2.14E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 *2 PLOG / 0.039 2.14E+80 -19.33 95177/ PLOG / 0.066 5.00E+68 -16.040 86832/ PLOG / 0.132 2.96E+59 -13.261 82596/ PLOG / 0.197 4.86E+61 -13.999 82637/ PLOG / 0.263 7.50E+59 -13.427 82179/ PLOG / 1.0E+5 2.92E+16 0.00 69120/

!C7H13 alkenyl reactions

P7XC7H13-1E (+M) = C2H4+P5XC5H9-1E (+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5/ TROE / -13.87 227 28 50000.0/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C7H12-16E+H(+M) = P7XC7H13-1E(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P7XC7H13-1E(+M) = S3XC7H13-1E(+M) 1.55E+02 2.83 15566.2 ! Ref to PXC6H11(+M) = S3XC6H11-1E(+M) LOW / 1.50E-30 14.56 -602.4/ TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S6XC7H13-1E(+M) = C4H7+C3H6(+M) 5.50E+11 0.55 28084.3 ! 08TSAb JetSurF 2.0 LOW/ 3.10E-43 18.418 -602.9 / TROE/ -32.13 207.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S6XC7H13-1E(+M) = S3XC7H13-1E(+M) 1.55E+02 2.83 15566.2 ! 08/TSwip JetSurF 2.0 LOW/ 1.50E-30 14.56 -602.4 / TROE/ -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C7H12-16E+H(+M) = S6XC7H13-1E(+M) 1.33E+13 0.00 1559.8 ! Ref to C4H8-1+H(+M) = sC4H9(+M) LOW / 8.70E+42 -7.50 4721.8/ TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C7H12-15E+H(+M) = S6XC7H13-1E(+M) 1.33E+13 0.00 1559.8 ! Ref to C4H8-2+H(+M) = sC4H9(+M) LOW / 8.70E+42 -7.50 4721.8 / TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC7H13-1E(+M) = C4H6+nC3H7(+M) 3.39E+11 0.66 32262.9 ! 08/TSAwip JetSurF 2.0 LOW/ 4.00E-42 18.045 -602.6 / TROE/ -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC7H13-1E(+M) = C7H12-13E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

P6XC6H10-1E4M(+M) = S4XC5H9-1E+C2H4(+M) 1.76E+11 0.57 28791.0 ! 08TSAa JetSurF 2.0 LOW/ 2.80E-44 18.729 -602.5 / TROE / -14.66 219.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C6H9-15E3M+H(+M) = P6XC6H10-1E4M(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E4M(+M) = S3XC6H10-1E4M(+M) 1.55E+02 2.83 15566.2 ! 08/TSwip JetSurF 2.0 LOW/ 1.50E-30 14.56 -602.4 / TROE/ -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H10-1E4M(+M) = C5H8-13E+C2H5(+M) 3.39E+11 0.66 31262.9 ! 08/TSAwip (-1 kcal/mol Ctert-Csec) JetSurF 2.0 LOW / 4.00E-42 18.045 -602.6/ TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H10-1E4M(+M) = C6H10-13E+CH3(+M) 3.39E+11 0.66 31262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.045 -602.6/ TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P7XC7H13-2E(+M) = S3XC5H9-1E+C2H4(+M) 9.12E+11 0.31 27237.8 ! 08TSAb (lumped C5H9) JetSurF 2.0 LOW / 1.80E-57 23.463 -602.4 / TROE/ -2.46 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C7H12-15E+H(+M) = P7XC7H13-2E(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P7XC7H13-2E(+M) = S4XC7H13-2E(+M) 1.55E+02 2.83 15566.2 ! 08/TSwip JetSurF 2.0 LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC7H13-2E(+M) = C5H8-13E+C2H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE/ -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC7H13-2E(+M) = C7H12-24E+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

S4XC7H13-2E(+M) = C7H12-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H LOW / 4.60E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

P6XC6H10-1E3M(+M) = P4XC4H6-1E3M+C2H4(+M) 2.38E+11 0.51 27281.5 ! 08TSAb JetSurF 2.0 LOW / 1.80E-57 23.463 -602.4 / TROE / -2.46 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C6H9-15E3M+H(+M) = P6XC6H10-1E3M(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E3M(+M) = T3XC6H10-1E3M(+M) 8.60E+01 2.62 8722.9 ! 08TSAc Est-2 JetSurF 2.0 LOW / 8.10E-33 15.214 -677.4/ TROE / -30.39 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

T3XC6H10-1E3M(+M) = C4H5-13E2M+C2H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE /-18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E5M(+M) = C4H7+C3H6(+M) 1.76E+11 0.57 28791.6 ! 08TSAc (2-methyl-pent-4-yl) JetSurF 2.0 LOW / 4.70E-39 16.77 -603.1/ TROE /-27.89 216 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E5M(+M) = C6H10-15E+CH3(+M) 1.76E+11 0.57 28791.6 ! 08TSAc (2-methyl-pent-4-yl) JetSurF 2.0 LOW / 4.70E-39 16.77 -603.1/ TROE/ -27.89 216 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C6H9-15E2M+H(+M) = P6XC6H10-1E5M(+M) 1.33E+13 0.00 3260.7 ! Ref to iC4H8+H(+M) = iC4H9(+M) LOW / 6.26E+38 -6.66 7000.0 / TROE / 1.000 1000 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E5M(+M) = S3XC6H10-1E5M(+M) 1.55E+02 2.83 15566.2 ! 08/TSwip JetSurF 2.0 LOW / 1.50E-30 14.56 -602.4 / TROE/ -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H10-1E5M(+M) = C4H6+iC3H7(+M) 3.39E+11 0.66 31262.9 ! 08/TSAwip (-1 kcal/mol Ctert-Csec) JetSurF 2.0 LOW / 4.00E-42 18.045 -602.6/ TROE /-18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H10-1E5M(+M) = C6H9-13E5M+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE /-51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

P6XC6H10-1E2M(+M) = P4XC4H6-1E2M+C2H4(+M) 3.98E+12 0.12 27571.6 ! 08/TSAwip JetSurF 2.0 LOW / 3.30E-43 18.35 -602.5 / TROE /-13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C6H9-15E2M+H(+M) = P6XC6H10-1E2M(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE / 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H10-1E2M(+M) = S3XC6H10-1E2M(+M) 1.55E+02 2.83 15566.2 ! 08/TSwip JetSurF 2.0 LOW / 1.50E-30 14.56 -602.4 / TROE /-13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC6H10-1E2M(+M) = C4H5-13E2M+C2H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

PXCH2cC6H11 = S3XMCH 2.30E+07 1.02 28687.0 ! PLOG / 0.039 2.30E+07 1.02 28687.0/ ! 4.65E+08 /20 EST PLOG / 1.000 4.65E+08 1.02 28687.0/ ! 09/SI-WA JetSurF 2.0

PXCH2cC6H11 = S4XMCH 6.0E+07 0.92 22700.0 ! PLOG / 0.039 6.0E+07 0.92 22700.0/ ! 1.19E+09 /20 EST PLOG / 1.000 1.19E+09 0.92 22700.0/ ! 09/SI-W JetSurF 2.0

PXCH2cC6H11=P7XC7H13-1E 8.92E+18 -2.94 19897 ! calculated in this work PLOG / 0.039 8.92E+18 -2.94 19897 / ! 800 K-2000 K PLOG / 0.197 6.83E+22 -3.82 23511 / ! 800 K-2000 K PLOG / 1.000 1.56E+29 -5.39 29211 / ! 800 K-2000 K PLOG / 10.000 4.15E+37 -7.44 37753 / ! 800 K-2000 K PLOG / 100.000 1.92E+39 -7.58 42286 / ! 800 K-2000 K PLOG / 1.0E+5 2.53E+13 0.16 29785 / ! 800 K-2000 K

PXCH2cC6H11=CH2cC6H10+H 8.14E+14 -2.42 21719 ! calculated in this work PLOG / 0.039 8.14E+14 -2.42 21719 / ! 800 K-2000 K PLOG / 0.197 1.23E+20 -3.61 26095 / ! 800 K-2000 K PLOG / 1.000 1.18E+28 -5.58 32946 / ! 800 K-2000 K PLOG / 10.000 1.31E+39 -8.28 43693 / ! 800 K-2000 K PLOG / 100.000 4.67E+42 -8.87 50298 / ! 800 K-2000 K PLOG / 1.0E+5 1.60E+11 0.59 35447 / ! 800 K-2000 K

T1XMCH=P6XC6H10-1E2M 7.77E+21 -3.78 22330 ! calculated in this work PLOG / 0.039 7.77E+21 -3.78 22330 / ! 800 K-2000 K PLOG / 0.197 2.46E+23 -3.98 24528 / ! 800 K-2000 K PLOG / 1.000 3.46E+31 -6.06 31348 / ! 800 K-2000 K PLOG / 10.000 3.04E+40 -8.25 40204 / ! 800 K-2000 K PLOG / 100.000 3.40E+43 -8.78 45692 / ! 800 K-2000 K PLOG / 1.0E+5 2.51E+13 0.24 31344 / ! 800 K-2000 K

T1XMCH=CH2cC6H10+H 5.68E+24 -4.98 28465 ! calculated in this work PLOG / 0.039 5.68E+24 -4.98 28465 / ! 800 K-2000 K PLOG / 0.197 4.63E+25 -4.97 30017 / ! 800 K-2000 K PLOG / 1.000 2.67E+34 -7.20 37107 / ! 800 K-2000 K PLOG / 10.000 4.39E+44 -9.70 46944 / ! 800 K-2000 K PLOG / 100.000 1.12E+49 -10.55 53815 / ! 800 K-2000 K PLOG / 1.0E+5 1.18E+14 -0.04 37343 / ! 800 K-2000 K

T1XMCH=MCH-1E+H 1.47E+22 -4.09 24874 ! calculated in this work PLOG / 0.039 1.47E+22 -4.09 24874 / ! 800 K-2000 K PLOG / 0.197 1.57E+23 -4.12 26671 / ! 800 K-2000 K PLOG / 1.000 7.83E+31 -6.33 33844 / ! 800 K-2000 K PLOG / 10.000 6.83E+41 -8.76 43572 / ! 800 K-2000 K PLOG / 100.000 7.93E+45 -9.52 50174 / ! 800 K-2000 K PLOG / 1.0E+5 5.80E+12 0.46 34881 / ! 800 K-2000 K

S2XMCH=P6XC6H10-1E3M 1.24E+22 -4.01 22066 ! calculated in this work PLOG / 0.039 1.24E+22 -4.01 22066 / ! 800 K-2000 K PLOG / 0.197 4.17E+22 -3.93 23430 / ! 800 K-2000 K PLOG / 1.000 1.01E+28 -5.23 28271 / ! 800 K-2000 K PLOG / 10.000 2.14E+37 -7.54 37062 / ! 800 K-2000 K PLOG / 100.000 1.11E+43 -8.81 44209 / ! 800 K-2000 K PLOG / 1.0E+5 1.59E+13 0.22 31118 / ! 800 K-2000 K

S2XMCH=P7XC7H13-2E 2.99E+22 -4.04 21843 ! calculated in this work PLOG / 0.039 2.99E+22 -4.04 21843 / ! 800 K-2000 K PLOG / 0.197 8.66E+22 -3.95 23164 / ! 800 K-2000 K PLOG / 1.000 1.44E+28 -5.21 27888 / ! 800 K-2000 K PLOG / 10.000 1.61E+37 -7.45 36452 / ! 800 K-2000 K PLOG / 100.000 4.39E+42 -8.66 43334 / ! 800 K-2000 K PLOG / 1.0E+5 2.37E+13 0.19 30429 / ! 800 K-2000 K

S2XMCH=MCH-1E+H 2.06E+20 -3.80 23117 ! calculated in this work PLOG / 0.039 2.06E+20 -3.80 23117 / ! 800 K-2000 K PLOG / 0.197 1.50E+21 -3.78 24651 / ! 800 K-2000 K PLOG / 1.000 2.14E+27 -5.27 30013 / ! 800 K-2000 K PLOG / 10.000 8.88E+37 -7.90 39841 / ! 800

K-2000 K PLOG / 100.000 9.49E+44 -9.50 48246 / ! 800 K-2000 K PLOG / 1.0E+5 5.69E+11 0.60 34004 / ! 800 K-2000 K

S2XMCH=MCH-2E+H 1.82E+20 -3.68 23447 ! calculated in this work PLOG / 0.039 1.82E+20 -3.68 23447 / ! 800 K-2000 K PLOG / 0.197 1.92E+21 -3.70 25053 / ! 800 K-2000 K PLOG / 1.000 5.62E+27 -5.27 30610 / ! 800 K-2000 K PLOG / 10.000 7.34E+38 -8.02 40816 / ! 800 K-2000 K PLOG / 100.000 2.67E+46 -9.75 49698 / ! 800 K-2000 K PLOG / 1.0E+5 2.01E+12 0.63 35196 / ! 800 K-2000 K

S2XMCH=cC6H10+CH3 4.24E+21 -3.89 22867 ! calculated in this work PLOG / 0.039 4.24E+21 -3.89 22867 / ! 800 K-2000 K PLOG / 0.197 2.58E+22 -3.86 24360 / ! 800 K-2000 K PLOG / 1.000 2.27E+28 -5.30 29571 / ! 800 K-2000 K PLOG / 10.000 4.14E+38 -7.84 39088 / ! 800 K-2000 K PLOG / 100.000 1.94E+45 -9.36 47105 / ! 800 K-2000 K PLOG / 1.0E+5 6.35E+13 0.20 33524 / ! 800 K-2000 K

S3XMCH=P6XC6H10-1E4M 1.21E+18 -2.84 19903 ! calculated in this work PLOG / 0.039 1.21E+18 -2.84 19903 / ! 800 K-2000 K PLOG / 0.197 7.98E+21 -3.70 23365 / ! 800 K-2000 K PLOG / 1.000 2.52E+28 -5.31 28978 / ! 800 K-2000 K PLOG / 10.000 8.05E+37 -7.66 38033 / ! 800 K-2000 K PLOG / 100.000 6.13E+42 -8.70 44718 / ! 800 K-2000 K PLOG / 1.0E+5 1.68E+13 0.21 31241 / ! 800 K-2000 K

S3XMCH=S6XC7H13-1E 5.23E+18 -2.93 19555 ! calculated in this work PLOG / 0.039 5.23E+18 -2.93 19555 / ! 800 K-2000 K PLOG / 0.197 2.06E+22 -3.73 22876 / ! 800 K-2000 K PLOG / 1.000 3.29E+28 -5.27 28275 / ! 800 K-2000 K PLOG / 10.000 3.31E+37 -7.49 36918 / ! 800 K-2000 K PLOG / 100.000 8.80E+41 -8.42 43157 / ! 800 K-2000 K PLOG / 1.0E+5 2.55E+13 0.17 30061 / ! 800 K-2000 K

S3XMCH=MCH-3E+H 1.19E+16 -2.44 20998 ! calculated in this work PLOG / 0.039 1.19E+16 -2.44 20998 / ! 800 K-2000 K PLOG / 0.197 5.50E+20 -3.50 24928 / ! 800 K-2000 K PLOG / 1.000 1.93E+28 -5.37 31247 / ! 800 K-2000 K PLOG / 10.000 3.19E+39 -8.14 41683 / ! 800 K-2000 K PLOG / 100.000 1.03E+46 -9.58 49952 / ! 800 K-2000 K PLOG / 1.0E+5 1.87E+12 0.63 34980 / ! 800 K-2000 K

S3XMCH=MCH-2E+H 6.78E+14 -2.23 21396 ! calculated in this work PLOG / 0.039 6.78E+14 -2.23 21396 / ! 800 K-2000 K PLOG / 0.197 8.10E+19 -3.39 25518 / ! 800 K-2000 K PLOG / 1.000 8.05E+27 -5.38 32106 / ! 800 K-2000 K PLOG / 10.000 6.73E+39 -8.33 43061 / ! 800 K-2000 K PLOG / 100.000 1.12E+47 -9.95 51964 / ! 800 K-2000 K PLOG / 1.0E+5 1.64E+12 0.61 36658 / ! 800 K-2000 K

S4XMCH=P6XC6H10-1E5M 1.26E+22 -3.85 22627 ! calculated in this work PLOG / 0.039 1.26E+22 -3.85 22627 / ! 800 K-2000 K PLOG / 0.197 3.57E+26 -4.89 26638 / ! 800 K-2000 K PLOG / 1.000 2.59E+32 -6.32 32020 / ! 800 K-2000 K PLOG / 10.000 2.07E+41 -8.51 40814 / ! 800 K-2000 K PLOG / 100.000 5.79E+44 -9.15 46530 / ! 800 K-2000 K PLOG / 1.0E+5 3.87E+13 0.20 31782 / ! 800 K-2000 K

S4XMCH=MCH-3E+H 8.38E+20 -3.63 23771 ! calculated in this work PLOG / 0.039 8.38E+20 -3.63 23771 / ! 800 K-2000 K PLOG / 0.197 8.32E+25 -4.80 28120 / ! 800 K-2000 K PLOG / 1.000 5.73E+32 -6.47 34206 / ! 800 K-2000 K PLOG / 10.000 1.37E+43 -9.02 44242 / ! 800 K-2000 K PLOG / 100.000 7.21E+47 -9.98 51272 / ! 800 K-2000 K PLOG / 1.0E+5 3.78E+12 0.63 34881 / ! 800 K-2000 K

!methylcyclohexane reactions

! H-abstractions of methylcyclohexane

MCH+H = PXCH2cC6H11+H2 6.66E+06 2.13 8894.8 ! calculated in this work MCH+H = T1XMCH+H2 4.53E+06 2.11 4098.6 ! calculated in this work MCH+H = S2XMCH+H2 2.08E+07 2.10 6474.4 ! calculated in this work MCH+H = S3XMCH+H2 2.07E+07 2.12 6441.2 ! calculated in this work MCH+H = S4XMCH+H2 1.16E+07 2.11 6339.1 ! calculated in this work MCH+CH3 = PXCH2cC6H11+CH4 3.75E+01 3.27 13516.0 ! 10LV JetSurF 2.0 MCH+CH3 = T1XMCH+CH4 1.91E+01 3.27 9022.0 ! 10LV JetSurF 2.0 MCH+CH3 = S2XMCH+CH4 6.68E+01 3.21 11418.0 ! 10LV JetSurF 2.0 MCH+CH3 = S3XMCH+CH4 7.18E+01 3.26 11303.0 ! 10LV JetSurF 2.0 MCH+CH3 = S4XMCH+CH4 1.82E+01 3.36 10931.0 ! 10LV JetSurF 2.0

! isomerization and decomposition of methylcyclohexane

MCH = cC6H11+CH3 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 1.85E+105 -26.15 129214 / PLOG / 0.0395 1.19E+92 -22.23 122595 / PLOG / 0.197 1.50E+80 -18.67 116938 / PLOG / 0.395 8.65E+63 -13.89 108211 / PLOG / 1 5.93E+64 -14.15 108486 / PLOG / 10 3.59E+45 -8.56 97430 / PLOG / 100 1.66E+33 -4.99 90100 / PLOG / 1.0E+5 1.10E+27 -3.20 86385 /

MCH = C7H14-1E 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 5.49E+115 -29.26 143180 / PLOG / 0.0395 1.03E+104 -25.68 138280 / PLOG / 0.197 1.92E+88 -20.96 130954 / PLOG / 0.395 3.07E+80 -18.65 126930 / PLOG / 1 5.57E+69 -15.49 121178 / PLOG / 10 4.90E+44 -8.17 107073 / PLOG / 100 7.98E+26 -3.02 96627 / PLOG / 1.0E+5 1.09E+17 -0.16 90732 /

MCH = C7H14-2E 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 9.52E+114 -28.98 140737 / PLOG / 0.0395 1.74E+103 -25.40 135829 / PLOG / 0.197 3.34E+87 -20.68 128511 / PLOG /

0.395 5.32E+79 -18.37 124487 / PLOG / 1 9.66E+68 -15.21 118735 / PLOG / 10 8.51E+43 -7.89 104630 / PLOG / 100 1.38E+26 -2.74 94184 / PLOG / 1.0E+5 1.90E+16 0.12 88289 /

MCH = C6H11-1E2M 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 2.25E+132 -34.10 155250 / PLOG / 0.0395 1.46E+109 -27.20 144350 / PLOG / 0.197 4.09E+93 -22.49 137505 / PLOG / 0.395 4.87E+85 -20.13 133555 / PLOG / 1 3.27E+74 -16.83 127710 / PLOG / 10 3.09E+47 -8.92 112705 / PLOG / 100 2.18E+27 -3.08 100948 / PLOG / 1.0E+5 6.04E+15 0.27 94051 /

MCH = C6H11-1E5M 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 1.99E+132 -34.11 154207 / PLOG / 0.0395 1.28E+109 -27.20 143306 / PLOG / 0.197 3.61E+93 -22.49 136462 / PLOG / 0.395 4.30E+85 -20.13 132511 / PLOG / 1 2.89E+74 -16.83 126667 / PLOG / 10 2.73E+47 -8.93 111662 / PLOG / 100 1.93E+27 -3.08 99905 / PLOG / 1.0E+5 5.34E+15 0.27 93008 /

MCH = C6H11-1E3M 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 1.70E+119 -30.34 147025 / PLOG / 0.0395 1.77E+108 -26.94 142902 / PLOG / 0.197 4.67E+92 -22.23 136004 / PLOG / 0.395 4.07E+107 -26.52 143245 / PLOG / 1 3.71E+73 -16.58 126164 / PLOG / 10 5.09E+46 -8.72 111220 / PLOG / 100 6.68E+26 -2.95 99619 / PLOG / 1.0E+5 2.53E+15 0.36 92802 /

MCH = C6H11-1E4M 1.00 0.00 0.00 ! 2013 Zhang et al. PLOG / 0.01 1.87E+119 -30.34 146825 / PLOG / 0.0395 1.95E+108 -26.95 142703 / PLOG / 0.197 5.13E+92 -22.24 135803 / PLOG / 0.395 4.47E+107 -26.52 143045 / PLOG / 1 4.07E+73 -16.58 125964 / PLOG / 10 5.59E+46 -8.72 111019 / PLOG / 100 7.33E+26 -2.95 99418 / PLOG / 1.0E+5 2.78E+15 0.35 92602 /

C7H14-1E = pC4H9+aC3H5 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C7H14-1E = C4H8-1+C3H6 7.08E+06 1.65 53752.0 ! PLOG / 0.039 3.54E+05 1.65 53752.0/ ! /20 EST PLOG / 1.0 7.08E+06 1.65 53752.0/ ! JetSurF 2.0

C7H14-1E+H = S3XC7H13-1E+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C7H14-1E+CH3 = S3XC7H13-1E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C7H14-2E = SAXC4H7+nC3H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177 / PLOG / 0.066 2.50E+68 -16.040 86832 / PLOG / 0.132

1.480E+59 -13.261 82596 / PLOG / 0.197 2.43E+61 -13.999 82637 / PLOG / 0.263 3.75E+59 -13.427 82179 / PLOG / 1.0E+5 1.46E+16 0.00 69120 /

C7H14-2E = C4H8-1+C3H6 1.42E+07 1.65 53752.0 ! PLOG / 0.039 7.0E+05 1.65 53752.0/ ! /20 EST PLOG / 1.0 1.42E+07 1.65 53752.0/ ! JetSurF 2.0

C7H14-2E+H = S3XC7H13-1E+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 C7H14-2E+CH3 = S3XC7H13-1E+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571 C7H14-2E+H = S4XC7H13-2E+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C7H14-2E+CH3 = S4XC7H13-2E+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H11-1E2M = iC4H7+nC3H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H11-1E2M = iC4H8+C3H6 7.08E+06 1.65 53752.0 ! EST, ref to C7H14-1E PLOG / 0.039 3.54E+05 1.65 53752.0/ ! PLOG / 1.0 7.08E+06 1.65 53752.0/ !

C6H11-1E2M+H = S3XC6H10-1E2M+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C6H11-1E2M+CH3 = S3XC6H10-1E2M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H11-1E5M = aC3H5+iC4H9 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H11-1E5M+H = S3XC6H10-1E5M+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C6H11-1E5M+CH3 = S3XC6H10-1E5M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H11-1E4M = aC3H5+sC4H9 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H11-1E4M = C3H6+C4H8-2 7.08E+06 1.65 53752.0 ! EST, ref to C7H14-1E PLOG / 0.039 3.54E+05 1.65 53752.0/ ! PLOG / 1.0 7.08E+06 1.65 53752.0/ !

C6H11-1E4M+H = S3XC6H10-1E4M+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C6H11-1E4M+CH3 = S3XC6H10-1E4M+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C6H11-1E3M = SAXC4H7+nC3H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H11-1E3M = S3XC6H11-1E+CH3 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

C6H11-1E3M = C4H8-2+C3H6 7.08E+06 1.65 53752.0 ! EST, ref to C7H14-1E PLOG / 0.039 3.54E+05 1.65 53752.0/ ! PLOG / 1.0 7.08E+06 1.65 53752.0/ !

C6H11-1E3M+H = T3XC6H10-1E3M+H2 2.65E+6 2.2 0.0 ! allylt LLNL-MI-407571 C6H11-1E3M+CH3 = T3XC6H10-1E3M+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

!!! ECH mechanism

! reactions of PAXCH2-2-1C4H7 (C5H9)

! PAXCH2-2-1C4H7 comes from C2H5-2-1C6H11

PAXCH2-2-1C4H7 = aC3H4+C2H5 2.00E+13 0.00 50078.0 ! PLOG / 0.039 1.00E+12 0.00 50078.0/ ! /20 EST PLOG / 1.0E+5 2.00E+13 0.00 50078.0/ ! 73/TSA JetSurF 2.0

! reactions of P1XC4H82M (C5H11)

! P1XC4H82M come from C7H13-1E5M

CH3+C4H8-1(+M) = P1XC4H82M(+M) 4.80E+10 0.00 8003.6 ! Ref to C3H6+CH3(+M) = iC4H9(+M) /2 LOW / 6.50E+27 -4.27 2431.1 / TROE / 0.565 60000.0 534.2 3007.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5+C3H6(+M) = P1XC4H82M(+M) 4.80E+10 0.00 8003.6 ! Ref to C3H6+CH3(+M) = iC4H9(+M) /2 LOW / 6.50E+27 -4.27 2431.1 / TROE / 0.565 60000.0 534.2 3007.2 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! reactions of C2H3-2-PXC4H6, C2H3-3-PXC4H6

C2H4+iC4H5 = C2H3-2-PXC4H6 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

C2H3+C4H6 = C2H3-3-PXC4H6 1.23E+35 -7.76 9930.0 ! Ref to C2H4+C2H3 = C4H7 PLOG / 0.039 6.15E+34 -7.76 9930.0 / PLOG / 0.1 1.23E+35 -7.76 9930.0 / PLOG / 1.0 7.93E+38 -8.47 14220.0/ PLOG / 10 2.99E+36 -7.40 15480.0/

!reactions of C6H11, P6XC6H11-2E, P5XC5H8-1E3M, P6XC6H11-3E, S4XC6H11-2E, PXCH2-3-1C5H9 !

! P6XC6H11-2E Come from P8XC8H15-2E

P6XC6H11-2E(+M) = SAXC4H7+C2H4(+M) 1.04E+12 -0.37 25124.2 ! 08/TSAwip LOW / 5.90E-31 13.982 -603.1 / TROE / -14.78 229 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH3S2XcC5H8=P6XC6H11-2E 4.27E+12 0.404 33710 ! HPL, 2-methylcyclopentyl radical decomposition, 2008 Sirjean et al. J. Phys. Chem. A 112 (2008) 11598-11610 CH3S2XcC5H8=P5XC5H8-1E3M 3.47E+10 0.959 33910 ! HPL, 2-methylcyclopentyl radical decomposition, 2008 Sirjean et al. J. Phys. Chem. A 112 (2008) 11598-11610 CH3S2XcC5H8=cC5H8+CH3 4.57E+11 0.843 30530 ! HPL, 2-methylcyclopentyl radical decomposition, 2008 Sirjean et al. J. Phys. Chem. A 112 (2008) 11598-11610

! P5XC5H8-1E3M Come from CH3S2XcC5H8 and P7XC7H12-1E3M

P5XC5H8-1E3M(+M) = SAXC4H7+C2H4(+M) 1.04E+12 -0.37 25124.2 ! Ref to P6XC6H11-2E LOW / 5.90E-31 13.982 -603.1 / TROE / -14.78 229 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! P6XC6H11-3E Come from P8XC8H15-3E

P6XC6H11-3E(+M) = C6H10-13E+H(+M) 4.27E+09 -0.96 31962.9 ! 08/TSwip LOW / 3.00E-45 13.55 -603.1 / TROE/ -35.89 249 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P6XC6H11-3E(+M) = S4XC6H11-2E(+M) 2.29E+01 2.82 10755.6 ! Ref to PXC8H17(+M) = S3XC8H17(+M), 1,5-H shift, in JetSurF 2.0, without considering the double bond LOW / 9.90E-38 17.215 -603.0 / TROE / -16.33 200.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC6H11-2E(+M) = C5H8-13E+CH3(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! P6XC6H11-3E Come from C2H5-3-PXC6H10

PXCH2-3-1C5H9(+M) = C4H6+C2H5(+M) 4.90E+12 0.15 11139.1 ! 08/TSAwip LOW / 1.70E-14 9.652 -603.1/ TROE / -76.60 221 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! reactions of C2H3cC5H9 (C7H12) !

C2H3cC5H9=C7H12-13E 2.45E20 -0.97 92860 ! Sirjean 2006 cyclopentane hpl, J. Phys. Chem. A 110 (2006) 12693-12704 PLOG / 0.039 1.25E19 -0.97 92860 / ! EST /20 PLOG / 1.0 2.45E20 -0.97 92860 / !

C2H3cC5H9+H = C2H3TXcC5H8+H2 2.65E+6 2.2 0.0 ! allylt LLNL-MI-407571 C2H3cC5H9+CH3 = C2H3TXcC5H8+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

C2H3cC5H9+H = C2H3S2XcC5H8+H2 2.60E+06 2.4 4471 ! secondary LLNL-MI-407571 x2 C2H3cC5H9+CH3 = C2H3S2XcC5H8+CH4 3.02E+00 3.46 5481 ! secondary LLNL-MI-407571 x2

C2H3cC5H9+H = C2H3S3XcC5H8+H2 2.60E+06 2.4 4471 ! secondary LLNL-MI-407571 x2 C2H3cC5H9+CH3 = C2H3S3XcC5H8+CH4 3.02E+00 3.46 5481 ! secondary LLNL-MI-407571 x2

C2H3TXcC5H8=C2H3-2-PXC5H8 1.86E+12 0.419 34370 ! 1-methylcyclopentyl radical sirjean 2008 hpl, J. Phys. Chem. A 112 (2008) 11598-11610 PLOG / 0.039 0.93E+11 0.419 34370 / ! EST /20 PLOG / 1.0 1.86E+12 0.419 34370 / !

C2H3-2-PXC5H8(+M) = P1XCH2C4H5-13E+C2H4(+M) 4.57E+12 0.13 24386.4 ! Ref S5XC6H11-1E(+M) = C3H6+aC3H5(+M) LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! to reduce the complex, only the ring opening to linear products were considered at present

C2H3S2XcC5H8=P7XC7H11-13E 4.27E+12 0.404 33710 ! 2-methylcyclopentyl radical sirjean 2008 hpl, J. Phys. Chem. A 112 (2008) 11598-11610 PLOG / 0.039 2.15E+11 0.404 33710 / ! EST /20 PLOG / 1.0 4.27E+12 0.404 33710/ !

C2H3S3XcC5H8=S3XC7H11-16E 1.44E+13 0.277 33740 ! 3-methylcyclopentyl radical sirjean 2008 hpl, J. Phys. Chem. A 112 (2008) 11598-11610 PLOG / 0.039 0.75E+12 0.277 33740 / ! EST /20 PLOG / 1.0 1.44E+13 0.277 33740/ !

P7XC7H11-13E(+M) = IC5H7+C2H4(+M) 4.57E+12 0.13 24386.4 ! Ref S5XC6H11-1E(+M) = C3H6+aC3H5(+M) LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! reactions of PAXCH2-2-1C6H11 (C7H13)

! PAXCH2-2-1C6H11 come from C2H5-2-1C6H11

PAXCH2-2-1C6H11 = aC3H4+pC4H9 2.00E+13 0.00 50078.0 ! PLOG / 0.039 1.00E+12 0.00 50078.0 / ! /20 EST PLOG / 1.0E+5 2.00E+13 0.00 50078.0 / ! 73/TSA JetSurF 2.0

! reactions of C8H12 chain dienes

! C2H3-2-1C6H11 come from CH3CH-2-1C6H11

C2H3-2-1C6H11=P1XCH2C4H5-13E+nC3H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 ! PLOG / 0.039 1.07E+80 -19.33 95177/ ! PLOG / 0.066 2.50E+68 -16.040 86832/ ! PLOG / 0.132 1.480E+59 -13.261 82596/ ! PLOG / 0.197 2.43E+61 -13.999 82637/ ! PLOG / 0.263 3.75E+59 -13.427 82179/ ! PLOG / 1.0E+5 1.46E+16 0.00 69120/ !

! reactions of cyclic C8H9

! CH2CH-1-SAXcC6H6 CH2CH-2-SAXcC6H6 CH2CH-3-SAXcC6H6 CH2CH-4-SAXcC6H6 CH2CH-5-SAXcC6H6

CH2CH-1-SAXcC6H6(+M)= A1C2H3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ CH2CH-2-SAXcC6H6(+M)= A1C2H3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ CH2CH-3-SAXcC6H6(+M)= A1C2H3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ CH2CH-4-SAXcC6H6(+M)= A1C2H3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ CH2CH-5-SAXcC6H6(+M)= A1C2H3+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

!reactions of cyclic C8H10

! CH2CH-1-cC6H7-13 CH2CH-2-cC6H7-13 CH3CH-5-cC6H6-13 CH3CH-3-cC6H6-14

CH2CH-1-cC6H7-13+H = CH2CH-1-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 CH2CH-1-cC6H7-13+CH3 = CH2CH-1-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2CH-1-SAXcC6H6+H(+M)=CH2CH-1-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2CH-1-cC6H7-13+H = CH2CH-4-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 CH2CH-1-cC6H7-13+CH3 = CH2CH-4-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2CH-4-SAXcC6H6+H(+M)=CH2CH-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2CH-2-cC6H7-13+H = CH2CH-2-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 CH2CH-2-cC6H7-13+CH3 = CH2CH-2-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2CH-2-SAXcC6H6+H(+M)=CH2CH-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2CH-2-cC6H7-13+H = CH2CH-3-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 CH2CH-2-cC6H7-13+CH3 = CH2CH-3-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH2CH-3-SAXcC6H6+H(+M)=CH2CH-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! ! reactions of cyclic C8H11

!CH2CH-2-SAXcC6H8 CH2CH-1-SAXcC6H8 CH3CH-3-PXcC6H7 CH3CH-6-SAXcC6H7 C2H5-1-SAXcC6H6 !C2H5-4-SAXcC6H6 CH3CH-1-cC6H7-13 C2H5-3-SAXcC6H6 C2H5-2-SAXcC6H6 CH3CH-2-cC6H7-13 !C2H5-6-SAXcC6H6 C2H5-5-SAXcC6H6

CH2CH-2-SAXcC6H8(+M)=CH2CH-2-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

CH2CH-1-SAXcC6H8(+M)=CH2CH-1-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-1-SAXcC6H6(+M)=A1C2H5+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-4-SAXcC6H6(+M)=A1C2H5+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

CH3CH-1-cC6H7-13(+M)=CH2CH-1-cC6H7-13+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW/ 4.61E-37 15.37 -603.1 / TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-3-SAXcC6H6(+M)= A1C2H5+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-2-SAXcC6H6(+M)= A1C2H5+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

CH3CH-2-cC6H7-13(+M)= CH2CH-2-cC6H7-13+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-6-SAXcC6H6(+M)=A1C2H5+H(+M) 1.56E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *1/3 LOW / 1.53E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-6-SAXcC6H6=A1+C2H5 4.24E+21 -3.89 22867 ! 800 K-2000 K ref to S2XMCH=cC6H10+CH3 PLOG / 0.039 4.24E+21 -3.89 22867/ PLOG / 0.197 2.58E+22 -3.86 24360/ PLOG / 1.000 2.27E+28 -5.30 29571/ PLOG / 10.000 4.14E+38 -7.84 39088/ PLOG / 100.000 1.94E+45 -9.36 47105/ PLOG / 1.0E+5 6.35E+13 0.20 33524/

C2H5-5-SAXcC6H6(+M)=A1C2H5+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-5-SAXcC6H6(+M)=CH2cC6H6-13E+CH3(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6/ TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!reactions of cyclic C8H12

C2H5-1-cC6H7-13+H = C2H5-1-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-1-cC6H7-13+CH3 = C2H5-1-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-1-SAXcC6H6+H(+M)=C2H5-1-cC6H7-13(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M *2/3 LOW / 0.89E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-1-cC6H7-13+H = C2H5-4-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-1-cC6H7-13+CH3 = C2H5-4-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-4-SAXcC6H6 + H(+M) = C2H5-1-cC6H7-13(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M *2/3 LOW / 0.89E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-1-cC6H7-13+H = CH3CH-1-cC6H7-13+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-1-cC6H7-13+CH3 = CH3CH-1-cC6H7-13+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH3CH-1-cC6H7-13 + H(+M) = C2H5-1-cC6H7-13(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M *2/3 LOW / 0.89E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2S4XcC6H7-5E+CH3(+M)=C2H5-1-cC6H7-13 (+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4 1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

C2H5-2-cC6H7-13+H = C2H5-3-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-2-cC6H7-13+CH3 = C2H5-3-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-3-SAXcC6H6+H(+M)=C2H5-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-2-cC6H7-13+H = C2H5-2-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-2-cC6H7-13+CH3 = C2H5-2-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-2-SAXcC6H6+H(+M)=C2H5-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-2-cC6H7-13+H = CH3CH-2-cC6H7-13+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-2-cC6H7-13+CH3 = CH3CH-2-cC6H7-13+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH3CH-2-cC6H7-13+H(+M)=C2H5-2-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2S2XcC6H7-5E+CH3(+M)=C2H5-2-cC6H7-13 (+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4 1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

C2H5-5-cC6H7-13+H = C2H5-6-SAXcC6H6+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571
C2H5-5-cC6H7-13+CH3 = C2H5-6-SAXcC6H6+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-6-SAXcC6H6+H(+M)=C2H5-5-cC6H7-13(+M) 1.33E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.89E+59 -12.00 5967.8/ TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-5-cC6H7-13+H = C2H5-5-SAXcC6H6+H2 2.65E+6 2.2 0.0 ! allylt LLNL-MI-407571
C2H5-5-cC6H7-13+CH3 = C2H5-5-SAXcC6H6+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

C2H5-5-SAXcC6H6+H(+M)=C2H5-5-cC6H7-13(+M) 0.67E+13 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *1/3 LOW / 0.44E+59 -12.00 5967.8/ TROE/ 0.020 1096.6 1096.6 6859.5/ H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S1XcC6H7-24E+C2H5(+M)=C2H5-5-cC6H7-13 (+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4H
1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

reactions of C2H3-2-PXC6H10, PXC8H13-13, C2H3-3-PXC6H10, SAXC8H13-17, C2H3-4-PXC6H10, C2H3-5-PXC6H10

C2H3-2-PXC6H10(+M) = C2H3-2-PXC4H6+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

PXC8H13-13(+M) = P6XC6H9-13E+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H3-3-PXC6H10(+M) = C2H3-3-PXC4H6+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

SAXC8H13-17(+M) = C4H6+C4H7(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H3-4-PXC6H10(+M) = S3XC6H9-15E+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H3-5-PXC6H10(+M) = C4H6+C4H7(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!CH2CH-1-cC6H10 CH2CH-2-cC6H10 CH2CH-3-cC6H10 CH2CH-4-cC6H10 CH3CH-2-cC6H9 C2H5-1-SAXcC6H8 C2H5-2-SAXcC6H8 CH3CH-1-cC6H9 !C2H5-6-SAXcC6H8 C2H5-3-SAXcC6H8 C2H5-4-SAXcC6H8 C2H5-5-SAXcC6H8

!! CH2CH-1-cC6H10 reactions

CH2CH-1-cC6H10=C2H3-2-PXC6H10 7.77E+21 -3.78 22330 ! Ref to T1XMCH=P6XC6H10-1E2M PLOG / 0.039 7.77E+21 -3.78 22330 / ! 800 K-2000 K PLOG / 0.197 2.46E+23 -3.98 24528 / ! 800 K-2000 K PLOG / 1.000 3.46E+31 -6.06 31348 / ! 800 K-2000 K PLOG / 10.000 3.04E+40 -8.25 40204 / ! 800 K-2000 K PLOG / 100.000 3.40E+43 -8.78 45692 / ! 800 K-2000 K PLOG / 1.0E+5 2.51E+13 0.24 31344 / ! 800 K-2000 K

!! CH2CH-2-cC6H10 reactions

CH2CH-2-cC6H10=C2H3-3-PXC6H10 1.24E+22 -4.01 22066 ! Ref to S2XMCH=P6XC6H10-1E3M PLOG / 0.039 1.24E+22 -4.01 22066 / ! 800 K-2000 K PLOG / 0.197 4.17E+22 -3.93 23430 / ! 800 K-2000 K PLOG / 1.000 1.01E+28 -5.23 28271 / ! 800 K-2000 K PLOG / 10.000 2.14E+37 -7.54 37062 / ! 800 K-2000 K PLOG / 100.000 1.11E+43 -8.81 44209 / ! 800 K-2000 K PLOG / 1.0E+5 1.59E+13 0.22 31118 / ! 800 K-2000 K

CH2CH-2-cC6H10=PXC8H13-13 2.99E+22 -4.04 21843 ! Ref to S2XMCH=P7XC7H13-2E PLOG / 0.039 2.99E+22 -4.04 21843 / ! 800 K-2000 K PLOG / 0.197 8.66E+22 -3.95 23164 / ! 800 K-2000 K PLOG / 1.000 1.44E+28 -5.21 27888 / ! 800 K-2000 K PLOG / 10.000 1.61E+37 -7.45 36452 / ! 800 K-2000 K PLOG / 100.000 4.39E+42 -8.66 43334 / ! 800 K-2000 K PLOG / 1.0E+5 2.37E+13 0.19 30429 / ! 800 K-2000 K

!! CH2CH-3-cC6H10 reactions

CH2CH-3-cC6H10=C2H3-4-PXC6H10 1.21E+18 -2.84 19903 ! Ref to S3XMCH=P6XC6H10-1E4M PLOG / 0.039 1.21E+18 -2.84 19903 / ! 800 K-2000 K PLOG / 0.197 7.98E+21 -3.70 23365 / ! 800 K-2000 K PLOG / 1.000 2.52E+28 -5.31 28978 / ! 800 K-2000 K PLOG / 10.000 8.05E+37 -7.66 38033 / ! 800 K-2000 K PLOG / 100.000 6.13E+42 -8.70 44718 / ! 800 K-2000 K PLOG / 1.0E+5 1.68E+13 0.21 31241 / ! 800 K-2000 K

CH2CH-3-cC6H10=SAXC8H13-17 5.23E+18 -2.93 19555 ! Ref to S3XMCH=S6XC7H13-1E PLOG / 0.039 5.23E+18 -2.93 19555 / ! 800 K-2000 K PLOG / 0.197 2.06E+22 -3.73 22876 / !

800 K-2000 K PLOG / 1.000 3.29E+28 -5.27 28275 / ! 800 K-2000 K PLOG / 10.000 3.31E+37 -7.49 36918 / ! 800 K-2000 K PLOG / 100.000 8.80E+41 -8.42 43157 / ! 800 K-2000 K PLOG / 1.0E+5 2.55E+13 0.17 30061 / ! 800 K-2000 K

!! CH2CH-4-cC6H10 reactions

CH2CH-4-cC6H10=C2H3-5-PXC6H10 1.26E+22 -3.85 22627 ! Ref to S4XMCH=P6XC6H10-1E5M PLOG / 0.039 1.26E+22 -3.85 22627 / ! 800 K-2000 K PLOG / 0.197 3.57E+26 -4.89 26638 / ! 800 K-2000 K PLOG / 1.000 2.59E+32 -6.32 32020 / ! 800 K-2000 K PLOG / 10.000 2.07E+41 -8.51 40814 / ! 800 K-2000 K PLOG / 100.000 5.79E+44 -9.15 46530 / ! 800 K-2000 K PLOG / 1.0E+5 3.87E+13 0.20 31782 / ! 800 K-2000 K

C2H5-1-SAXcC6H8(+M)=C2H5-1-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-2-SAXcC6H8(+M)=C2H5-2-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-6-SAXcC6H8(+M)=C2H5-5-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE /-51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-3-SAXcC6H8(+M)=C2H5-2-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M *2/3 LOW / 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

C2H5-3-SAXcC6H8=CH2cC6H8-2E+CH3 1.17E+22 -3.78 22330 ! EST, C2H5TXcC6H10=C2H5-2-PXC6H10 *1.5, fall off from C2H5TXcC6H10=C2H5-2-PXC6H10. PLOG / 0.039 1.17E+22 -3.78 22330 / PLOG / 0.197 3.69E+23 -3.98 24528 / PLOG / 1.000 5.19E+31 -6.06 31348 / PLOG / 10.000 4.56E+40 -8.25 40204 / PLOG / 100.000 5.10E+43 -8.78 45692 / PLOG / 1.0E+5 3.77E+13 0.24 31344 /

C2H5-4-SAXcC6H8=cC6H8-13E+C2H5 1.06E+22 -3.89 22867 ! 800 K-2000 K ref to C2H5S2XcC6H10=cC6H1 PLOG / 0.039 1.06E+22 -3.89 22867 / PLOG / 0.197 6.45E+22 -3.86 24360 / PLOG / 1.000 5.68E+28 -5.30 29571 / PLOG / 10.000 1.04E+39 -7.84 39088 / PLOG / 100.000 4.85E+45 -9.36 47105 / PLOG / 1.0E+5 1.59E+14 0.20 33524 /

C2H5-4-SAXcC6H8=C2H5-1-cC6H7-13+H 2.06E+20 -3.80 23117 ! 800 K-2000 K ref to S2XMCH=MCH-1E+H PLOG / 0.039 2.06E+20 -3.80 23117 / PLOG / 0.197 1.50E+21 -3.78 24651 / PLOG /

1.000 2.14E+27 -5.27 30013 / PLOG / 10.000 8.88E+37 -7.90 39841 / PLOG / 100.000 9.49E+44 -9.50 48246 / PLOG / 1.0E+5 5.69E+11 0.60 34004 /

C2H5-5-SAXcC6H8(+M)=C2H5-5-cC6H7-13+H(+M) 3.13E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M *2/3 LOW/ 3.07E-37 15.37 -603.1/ TROE/ -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

reactions of C8H14-13E

C8H14-13E+H = C6H12-1E+C2H3 1.46E+30 -4.34 21647.0 ! =(C4H6+H) C8H14-13E= nC3H7+lC5H7 1.07E+80 -19.33 95177 ! Ref to C6H12-1E=aC3H5+nC3H7 PLOG / 0.039 1.07E+80 -19.33 95177/ PLOG / 0.066 2.50E+68 -16.040 86832/ PLOG / 0.132 1.480E+59 -13.261 82596/ PLOG / 0.197 2.43E+61 -13.999 82637/ PLOG / 0.263 3.75E+59 -13.427 82179/ PLOG / 1.0E+5 1.46E+16 0.00 69120/

reactions of cyclic C8H14

!CH2CHcC6H11 CH3CHcC6H10 C2H5-1-cC6H9 C2H5-3-cC6H9 C2H5-4-cC6H9

! CH2CHcC6H11 reactions CH2CHcC6H11=C8H14-13E 1.00 0.00 0.00 ! Ref to MCH = C7H14-2E, without considering the allylic resonance PLOG / 0.01 9.52E+114 -28.98 140737 / PLOG / 0.0395 1.74E+103 -25.40 135829 / PLOG / 0.197 3.34E+87 -20.68 128511 / PLOG / 0.395 5.32E+79 -18.37 124487 / PLOG / 1 9.66E+68 -15.21 118735 / PLOG / 10 8.51E+43 -7.89 104630 / PLOG / 100 1.38E+26 -2.74 94184 / PLOG / 1.0E+5 1.90E+16 0.12 88289 /

CH2CH-1-cC6H10+H(+M) = CH2CHcC6H11(+M) 2.00E+14 0.00 0.0 ! EST From C4H8-1 LOW / 2.66E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2CHcC6H11+H = CH2CH-1-cC6H10+H2 2.65E6 2.2 0.0 ! allylt LLNL-MI-407571 CH2CHcC6H11+CH3 = CH2CH-1-cC6H10+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

CH2CHcC6H11+H=CH2CH-2-cC6H10+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 CH2CHcC6H11+CH
2-cC6H10+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

CH2CHcC6H11+H=CH2CH-3-cC6H10+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 CH2CHcC6H11+CH
3-cC6H10+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

CH2CHcC6H11+H=CH2CH-4-cC6H10+H2 1.3E06 2.4 4471 ! secondary LLNL-MI-407571 CH2CHcC6H11+CH
4-cC6H10+CH4 1.51 3.46 5481 ! secondary LLNL-MI-407571

! CH3CHcC6H10 reactions

CH3CHcC6H10+H = CH2CH-1-cC6H10+H2 1.73E5 2.5 2492 ! allylp LLNL-MI-407571 CH3CHcC6H10+CH3 = CH2CH-1-cC6H10+CH4 2.2098 3.5 5675 ! allylp LLNL-MI-407571

CH2CH-1-cC6H10+H(+M)=CH3CHcC6H10(+M) 2.00E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) LOW / 1.35E+60 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! C2H5-1-cC6H9 reactions

C2H5-1-cC6H9+H = C2H5-1-SAXcC6H8+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-1-cC6H9+CH3 = C2H5-1-SAXcC6H8+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-1-SAXcC6H8+H(+M)=C2H5-1-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.90E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-1-cC6H9+H = C2H5-2-SAXcC6H8+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-1-cC6H9+CH3 = C2H5-2-SAXcC6H8+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-2-SAXcC6H8+H(+M) = C2H5-1-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.90E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-1-cC6H9+H = CH3CH-1-cC6H9+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-1-cC6H9+CH3 = CH3CH-1-cC6H9+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

CH3CH-1-cC6H9+H(+M) = C2H5-1-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.90E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2S2XcC6H9+CH3(+M)=C2H5-1-cC6H9(+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4H8-1(+M) LOW / 3.51E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

! C2H5-3-cC6H9 reactions

C2H5-3-cC6H9+H = C2H5-6-SAXcC6H8+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-3-cC6H9+CH3 = C2H5-6-SAXcC6H8+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-6-SAXcC6H8+H(+M)=C2H5-3-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW/ 0.90E+60 -12.00 5967.8 / TROE /0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-3-cC6H9+H = C2H5-3-SAXcC6H8+H2 2.65E+6 2.2 0.0 ! allylt LLNL-MI-407571 C2H5-3-cC6H9+CH3 = C2H5-3-SAXcC6H8+CH4 4.613 3.1 2330 ! allylt LLNL-MI-407571

C2H5-3-SAXcC6H8+H(+M)=C2H5-3-cC6H9(+M) 0.67E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) /3 LOW / 0.44E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XcC6H9-1E+C2H5(+M)=C2H5-3-cC6H9 (+M) 1.00E+14 -0.32 -262. ! Ref to aC3H5+CH3(+M)=C4H8-1(+M) Tsang 91 LOW / 3.5E+60 -12.97 6000./ TROE / 0.896 60000 1606 6118/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/

C2H5-3-cC6H9=C6H10-13E+C2H4 5.0E+78 -18.94 98386 ! ref to cC6H10 = C4H6+C2H4 PLOG / 0.039 5.0E+78 -18.94 98386 / PLOG / 0.197 2.60E+70 -16.36 95510 / PLOG / 1.0 3.81E+25 -3.58 64034 / PLOG / 1.0E+5 8.31E+13 0.387 64116 /

! C2H5-4-cC6H9 reactions

C2H5-4-cC6H9+H = C2H5-4-SAXcC6H8+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-4-cC6H9+CH3 = C2H5-4-SAXcC6H8+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-4-SAXcC6H8+H(+M)=C2H5-4-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.90E+60 -12.00 5967.8 / TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-4-cC6H9+H = C2H5-5-SAXcC6H8+H2 3.376E+5 2.36 207 ! allyls LLNL-MI-407571 C2H5-4-cC6H9+CH3 = C2H5-5-SAXcC6H8+CH4 3.69 3.31 4002 ! allyls LLNL-MI-407571

C2H5-5-SAXcC6H8+H(+M)=C2H5-4-cC6H9(+M) 1.33E+14 0.00 0.0 ! Ref to aC3H5+H(+M) = C3H6(+M) *2/3 LOW / 0.90E+60 -12.00 5967.8 / TROE/ 0.020 1096.6 1096.6 6859.5 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-4-cC6H9=C4H8-1+C4H6 5.0E+78 -18.94 98386 ! ref to cC6H10 = C4H6+C2H4 PLOG / 0.039 5.0E+78 -18.94 98386 / PLOG / 0.197 2.60E+70 -16.36 95510 / PLOG / 1.0 3.81E+25 -3.58 64034 / PLOG / 1.0E+5 8.31E+13 0.387 64116 /

C2H5-4-cC6H9 = S3XcC6H9-1E+C2H5 1.00 0.00 0.00 ! Ref to MCH = cC6H11+CH3 PLOG / 0.01 1.85E+105 -26.15 129214 / PLOG / 0.0395 1.19E+92 -22.23 122595 / PLOG / 0.197 1.50E+80 -18.67 116938 / PLOG / 0.395 8.65E+63 -13.89 108211 / PLOG / 1 5.93E+64 -14.15 108486 / PLOG / 10 3.59E+45 -8.56 97430 / PLOG / 100 1.66E+33 -4.99 90100 / PLOG / 1.0E+5 1.10E+27 -3.20 86385 /

C8H15 alkenyl reactions

!!! P8XC8H15-2E reaction

P8XC8H15-2E(+M) = P6XC6H11-2E+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P8XC8H15-2E(+M) = S4XC8H15-2E(+M) 2.29E+01 2.82 10755.6 ! Ref to PXC8H17(+M) = S3XC8H17(+M), 1,5-H shift, without consideration of allylic resonance, in JetSurF 2.0 LOW / 9.90E-38 17.215 -603.0 / TROE / -16.33 200.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC8H15-2E(+M) = C5H8-13E+nC3H7(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S4XC8H15-2E(+M) = C8H14-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

! P7XC7H12-1E3M reaction

P7XC7H12-1E3M(+M) = P5XC5H8-1E3M+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P7XC7H12-1E3M(+M) = T3XC7H12-1E3M(+M) 2.29E+01 2.82 10755.6 ! est LOW / 9.90E-38 17.215 -603.0 / TROE / -16.33 200.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

T3XC7H12-1E3M(+M) = C4H5-13E2M+nC3H7(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!!! C2H5-2-PXC6H10 reaction

C2H5-2-PXC6H10(+M) = PXC2H4-2-1C4H7+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-2-PXC6H10(+M) = C2H5-2-SAX1C6H10(+M) 1.55E+02 2.83 15566.2 ! Ref to P6XC6H11-1E(+M) = S3XC6H11-1E(+M) LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!! CH3CH-2-1C6H11 reaction

C2H5-2-PXC6H10(+M) = CH3CH-2-1C6H11(+M) 2.95E+00 3.08 11015.9 ! Ref to PXC8H17(+M) = S2XC8H17(+M) 1,6-H shift,without consideration of allylic resonance, in JetSurF 2.0 LOW / 3.90E-34 15.855 -606.2 / TROE / -15.24 216.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH3CH-2-1C6H11(+M) = C2H3-2-1C6H11+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7(+M) = C4H6+H(+M) LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

CH3CH-2-1C6H11 = C4H612+pC4H9 7.10E+10 1.38 56360 ! Ref to iC4H7=aC3H4+CH3, HPL, 2005 Zheng et al. J. Phys. Chem. A, 109 (2005) 9044 - 9053 PLOG / 0.039 3.55E+09 1.38 56360 / ! EST/20 PLOG / 1.0 7.10E+10 1.38 56360 /

!! PXCH2(C2H5)cC5H8 reaction

!!! C2H5-3-PXC6H10 reaction

! not refer to pxc6h11 C2H5-3-PXC6H10(+M) = PXCH2-3-1C5H9+C2H4(+M) 9.12E+11 0.31 27237.8 ! 08TSAb JetSurF 2.0 LOW / 1.80E-57 23.463 -602.4/ TROE / -2.46 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-3-PXC6H10(+M) = C2H5-3-TAX1C6H10(+M) 8.60E+01 2.62 8722.9 ! 08TSAc Est-2 JetSurF 2.0 LOW / 8.10E-33 15.214 -677.4 / TROE / -30.39 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-3-TAX1C6H10(+M) = CH2-3-C6H10-1E+CH3(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!! C3H7-3-SXC5H8 reaction

C2H5-3-PXC6H10(+M) = C3H7-3-SXC5H8(+M) 2.29E+01 2.82 10755.6 ! Ref to PXC8H17(+M) = S3XC8H17(+M), 1,5-H shift, in JetSurF 2.0 LOW / 9.90E-38 17.215 -603.0 / TROE / -16.33 200.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C3H7-3-SXC5H8(+M) = C5H8-13E+nC3H7(+M) 4.47E+11 0.57 28044.5 ! SXC6H13(+M) = C3H6+nC3H7(+M) in JetSurF 2.0 LOW / 3.70E-33 14.91 -600.0 / TROE / -6.53 333.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! C2H5-3-SXC6H10 reaction

C3H7-3-SXC5H8(+M) = C2H5-3-SXC6H10(+M) 1.41E+00 3.32 16144.4 ! Ref to SXC8H17(+M) = S3XC8H17(+M), 1,4-H shift in JetSurF 2.0 LOW / 5.20E-30 14.079 -606.4 / TROE / -21.93 219.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-3-SXC6H10(+M) = S3XC5H9-1E+C3H6(+M) 4.57E+12 0.13 24386.4 ! Ref to S5XC6H11-1E(+M) = C3H6+aC3H5(+M) in JetSurF 2.0 LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! P8XC8H15-4E reaction

P8XC8H15-4E(+M) = S3XC6H11-1E+C2H4(+M) 4.57E+12 0.13 24386.4 ! Ref to S5XC6H11-1E(+M) = C3H6+aC3H5(+M) in JetSurF 2.0 LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P8XC8H15-4E(+M) = S5XC8H15-3E(+M) 2.95E+00 3.08 11015.9 ! Ref to PXC8H17(+M) = S2XC8H17(+M), 1,6-H shift, without consideration of allylic resonance, in JetSurF 2.0 LOW / 3.90E-34 15.855 -606.2/ TROE / -15.24 216.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! C2H5-3-S2XC6H10 reaction

C2H5-3-S2XC6H10(+M) = C6H10-13E+C2H5(+M) 3.55E+12 0.29 28296.9 ! Ref to S2XC6H13(+M) = C2H5+C4H81(+M) in JetSurF 2.0 LOW / 4.50E-26 13.09 -600.5 / TROE / -0.74 308.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P8XC8H15-3E(+M) = P6XC6H11-3E+C2H4(+M) 9.12E+11 0.31 27237.8 ! 08TSAb LOW / 1.80E-57 23.463 -602.4 / TROE / -2.46 206.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

P8XC8H15-3E(+M) = S5XC8H15-3E(+M) 1.46E+11 0.00 10516.8 ! Est-2 LOW / 9.90E-38 17.215 -603.0 / TROE / -16.33 200.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S5XC8H15-3E(+M) = C6H10-13E+C2H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S5XC8H15-3E(+M) = C7H12-13E+CH3(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!!! reactions of PXC2H4-4-1C6H11

PXC2H4-4-1C6H11(+M) = S4XC6H11-1E+C2H4(+M) 3.98E+12 0.12 27571.6 ! Ref to P6XC6H11-1E(+M) = C4H7+C2H4(+M) LOW / 3.30E-43 18.35 -602.5 / TROE / -13.87 227 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

PXC2H4-4-1C6H11(+M) = C2H5-4-SAX1C6H10(+M) 1.55E+02 2.83 15566.2 ! Ref to P6XC6H11-1E(+M) = S3XC6H11-1E(+M) LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-4-SAX1C6H10(+M) = C6H10-13E+C2H5(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!!! reactions of C2H5-4-SXC6H10

PXC2H4-4-1C6H11(+M) = C2H5-4-SXC6H10(+M) 5.13E+00 3.23 16847.8 ! Ref to PXC8H17(+M) = S3XC8H17(+M), 1,4-H shift, in JetSurF 2.0 LOW / 5.10E-44 18.749 -602.9 / TROE / -20.15 205.0 28.0 5000000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-4-SXC6H10(+M) = C5H10-2E+aC3H5(+M) 4.57E+12 0.13 24386.4 ! Ref to S5XC6H11-1E(+M) = C3H6+aC3H5(+M) LOW / 2.50E-31 14.57 -578.8 / TROE / -13.17 268 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5-4-SXC6H10(+M) = C6H10-14E+C2H5(+M) 1.76E+11 0.57 28791.6 ! Ref to 08TSAc (2-methyl-pent-4-yl) LOW / 4.70E-39 16.77 -603.1/ TROE / -27.89 216 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!!! reactions of S6XC8H15-1E

S6XC8H15-1E(+M) = C4H7+C4H8-1(+M) 2.04E+13 0.04 28493.6 ! Ref to S2XC8H17(+M) = pC4H9+C4H81(+M) LOW / 3.00E-43 18.430 -602.8 / TROE / -34.47 208.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S6XC8H15-1E(+M) = C7H12-16E+CH3(+M) 9.55E+09 1.08 29387.7 ! Ref to S2XC8H17(+M) = C7H14+CH3(+M) LOW / 5.30E-46 19.133 -602.7 / TROE / -34.36 210.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S6XC8H15-1E(+M) = S3XC8H15-1E(+M) 1.55E+02 2.83 15566.2 ! Ref to P6XC6H11-1E(+M) = S3XC6H11-1E(+M) LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC8H15-1E(+M) = C4H6+pC4H9(+M) 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.05 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC8H15-1E(+M) = C8H14-13E+H(+M) 4.70E+08 1.32 44697.6 ! Ref to SAXC4H7 = C4H6 + H LOW / 4.6E-37 15.37 -603.1/ TROE / -51.87 258 28 50000.0 / H2/2/ CH4/2/ C2H6/3/

!!! Reactions of PXCH2-5-1C7H13

PXCH2-5-1C7H13(+M) = C4H7+C4H8-1(+M) 1.76E+11 0.57 28791.6 ! 08TSAc LOW / 4.70E-39 16.77 -603.1/ TROE / -27.89 216 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

PXCH2-5-1C7H13(+M) = C6H10-15E+C2H5(+M) 1.76E+11 0.57 28791.6 ! 08TSAc (2-methyl-pent-4-yl) LOW / 4.70E-39 16.77 -603.1/ TROE / -27.89 216 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

PXCH2-5-1C7H13(+M) = S3XC7H12-1E5M(+M) 1.55E+02 2.83 15566.2 ! Ref to P6XC6H11-1E(+M) = S3XC6H11-1E(+M) LOW / 1.50E-30 14.56 -602.4 / TROE / -13.59 214 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

S3XC7H12-1E5M(+M) = C4H6+sC4H9(+M) 3.39E+11 0.66 31262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) LOW / 4.00E-42 18.045 -602.6 / TROE / -18.50 246 28 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

!Ethylcyclohexane radical reactions

PXC2H4cC6H11 = C2H5S2XcC6H10 4.58E+08 0.90 22900.0 ! 09/SI-WA JetSurF 2.0 PLOG / 0.039 2.29E+07 0.90 22900.0/ ! /20 EST PLOG / 1.0 4.58E+08 0.90 22900.0/ !

PXC2H4cC6H11 = C2H5S3XcC6H10 4.94E+08 0.78 18644.0 ! 09/SI-WA JetSurF 2.0 PLOG / 0.039 2.47E+07 0.78 18644.0/ ! /20 EST PLOG / 1.0 4.94E+08 0.78 18644.0/ !

PXC2H4cC6H11 = C2H5S4XcC6H10 7.97E+08 0.78 22740.0 ! 09/SI-WA JetSurF 2.0 PLOG / 0.039 4.00E+07 0.78 22740.0/ ! /20 EST PLOG / 1.0 7.97E+08 0.78 22740.0/ !

SXC2H4cC6H11 = C2H5S3XcC6H10 4.65E+08 1.02 28687.0 ! 09/SI-WA JetSurF 2.0 PLOG / 0.039 2.33E+07 1.02 28687.0/ ! /20 EST PLOG / 1.0 4.65E+08 1.02 28687.0/ !

SXC2H4cC6H11 = C2H5S4XcC6H10 1.19E+09 0.92 22700.0 ! 09/SI-WA JetSurF 2.0 PLOG / 0.039 5.95E+07 0.92 22700.0/ ! /20 EST PLOG / 1.0 1.19E+09 0.92 22700.0/ !

PXC2H4cC6H11(+M) = cC6H11+C2H4(+M) 6.03E+10 0.84 27820.0 ! 08TSAb LOW / 1.00E-43 18.591 -602.5/ TROE/ -43.32 200.0 28.0 50000.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

CH2CHcC6H11+H(+M)=PXC2H4cC6H11(+M) 1.33E+13 0.00 3260.7 ! Ref to C3H6+H(+M) = nC3H7(+M) LOW / 6.26E+38 -6.66 7000.0/ TROE/ 1.000 1000.0 1310.0 48097.0 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

SXC2H4cC6H11=P8XC8H15-2E 8.92E+18 -2.94 19897 ! Ref to PXCH2cC6H11=P7XC7H13-1E PLOG / 0.039 8.92E+18 -2.94 19897 / ! 800 K-2000 K PLOG / 0.197 6.83E+22 -3.82 23511 /

! 800 K-2000 K PLOG / 1.000 1.56E+29 -5.39 29211 / ! 800 K-2000 K PLOG / 10.000 4.15E+37 -7.44 37753 / ! 800 K-2000 K PLOG / 100.000 1.92E+39 -7.58 42286 / ! 800 K-2000 K PLOG / 1.0E+5 2.53E+13 0.16 29785 / ! 800 K-2000 K

CH2CHcC6H11+H(+M) = SXC2H4cC6H11(+M) 6.65E+12 0.00 1559.8 ! Ref to C3H6+H(+M) = iC3H7(+M) /2 LOW / 4.35E+42 -7.50 4721.8/ TROE / 1.000 1000.0 645.4 6844.3 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

C2H5TXcC6H10=CH2cC6H10+CH3 8.20E+18 -2.83 21257 ! HPL est 2-methyl-2-butyl radical, 2006 Curran, Int. J. Chem. Kinet. 38 (2006) 250-275, fall off from C2H5TXcC6H10=C2H5-2-PXC6H10. PLOG / 0.039 8.20E+18 -2.83 21257 / PLOG / 0.197 2.60E+20 -3.03 23458 / PLOG / 1.000 3.65E+28 -5.11 30284 / PLOG / 10.000 3.21E+37 -7.30 39149 / PLOG / 100.000 3.59E+40 -7.83 44643 / PLOG / 1.0E+5 2.65E+10 1.19 30280 /

C2H5TXcC6H10=C2H5-2-PXC6H10 7.77E+21 -3.78 22330 ! Ref to T1XMCH=P6XC6H10-1E2M PLOG / 0.039 7.77E+21 -3.78 22330 / ! 800 K-2000 K PLOG / 0.197 2.46E+23 -3.98 24528 / ! 800 K-2000 K PLOG / 1.000 3.46E+31 -6.06 31348 / ! 800 K-2000 K PLOG / 10.000 3.04E+40 -8.25 40204 / ! 800 K-2000 K PLOG / 100.000 3.40E+43 -8.78 45692 / ! 800 K-2000 K PLOG / 1.0E+5 2.51E+13 0.24 31344 / ! 800 K-2000 K

C2H5TXcC6H10=CH3CHcC6H10+H 7.35E+21 -4.09 24874 ! EST C2H5TXcC6H10=C2H5-1-cC6H9+H /2 PLOG / 0.039 7.35E+21 -4.09 24874 / PLOG / 0.197 7.85E+22 -4.12 26671 / PLOG / 1.000 3.92E+31 -6.33 33844 / PLOG / 10.000 3.42E+41 -8.76 43572 / PLOG / 100.000 3.97E+45 -9.52 50174 / PLOG / 1.0E+5 2.90E+12 0.46 34881 /

C2H5TXcC6H10=C2H5-1-cC6H9+H 1.47E+22 -4.09 24874 ! Ref to T1XMCH=MCH-1E+H PLOG / 0.039 1.47E+22 -4.09 24874 / ! 800 K-2000 K PLOG / 0.197 1.57E+23 -4.12 26671 / ! 800 K-2000 K PLOG / 1.000 7.83E+31 -6.33 33844 / ! 800 K-2000 K PLOG / 10.000 6.83E+41 -8.76 43572 / ! 800 K-2000 K PLOG / 100.000 7.93E+45 -9.52 50174 / ! 800 K-2000 K PLOG / 1.0E+5 5.80E+12 0.46 34881 / ! 800 K-2000 K

C2H5S2XcC6H10= C2H5-3-PXC6H10 1.24E+22 -4.01 22066 ! Ref to S2XMCH=P6XC6H10-1E3M PLOG / 0.039 1.24E+22 -4.01 22066 / ! 800 K-2000 K PLOG / 0.197 4.17E+22 -3.93 23430 / ! 800 K-2000 K PLOG / 1.000 1.01E+28 -5.23 28271 / ! 800 K-2000 K PLOG / 10.000 2.14E+37 -7.54 37062 / ! 800 K-2000 K PLOG / 100.000 1.11E+43 -8.81 44209 / ! 800 K-2000 K PLOG / 1.0E+5 1.59E+13 0.22 31118 / ! 800 K-2000 K

C2H5S2XcC6H10= P8XC8H15-3E 2.99E+22 -4.04 21843 ! Ref to S2XMCH=P7XC7H13-2E PLOG / 0.039 2.99E+22 -4.04 21843 / ! 800 K-2000 K PLOG / 0.197 8.66E+22 -3.95 23164 / !

800 K-2000 K PLOG / 1.000 1.44E+28 -5.21 27888 / ! 800 K-2000 K PLOG / 10.000 1.61E+37 -7.45 36452 / ! 800 K-2000 K PLOG / 100.000 4.39E+42 -8.66 43334 / ! 800 K-2000 K PLOG / 1.0E+5 2.37E+13 0.19 30429 / ! 800 K-2000 K

C2H5S2XcC6H10=C2H5-1-cC6H9+H 2.06E+20 -3.80 23117 ! Ref to S2XMCH=MCH-1E+H PLOG / 0.039 2.06E+20 -3.80 23117 / ! 800 K-2000 K PLOG / 0.197 1.50E+21 -3.78 24651 / ! 800 K-2000 K PLOG / 1.000 2.14E+27 -5.27 30013 / ! 800 K-2000 K PLOG / 10.000 8.88E+37 -7.90 39841 / ! 800 K-2000 K PLOG / 100.000 9.49E+44 -9.50 48246 / ! 800 K-2000 K PLOG / 1.0E+5 5.69E+11 0.60 34004 / ! 800 K-2000 K

C2H5S2XcC6H10=C2H5-3-cC6H9+H 1.82E+20 -3.68 23447 ! Ref to S2XMCH=MCH-2E+H PLOG / 0.039 1.82E+20 -3.68 23447 / ! 800 K-2000 K PLOG / 0.197 1.92E+21 -3.70 25053 / ! 800 K-2000 K PLOG / 1.000 5.62E+27 -5.27 30610 / ! 800 K-2000 K PLOG / 10.000 7.34E+38 -8.02 40816 / ! 800 K-2000 K PLOG / 100.000 2.67E+46 -9.75 49698 / ! 800 K-2000 K PLOG / 1.0E+5 2.01E+12 0.63 35196 / ! 800 K-2000 K

C2H5S2XcC6H10= cC6H10+C2H5 4.24E+21 -3.89 20767 ! Ref to S2XMCH=cC6H10+CH3, energy barrier reduced 2.1 kcal/mol PLOG / 0.039 4.24E+21 -3.89 20767 / ! 800 K-2000 K PLOG / 0.197 2.58E+22 -3.86 22260 / ! 800 K-2000 K PLOG / 1.000 2.27E+28 -5.30 27471 / ! 800 K-2000 K PLOG / 10.000 4.14E+38 -7.84 36988 / ! 800 K-2000 K PLOG / 100.000 1.94E+45 -9.36 45005 / ! 800 K-2000 K PLOG / 1.0E+5 6.35E+13 0.20 31424 / ! 800 K-2000 K

C2H5S3XcC6H10= PXC2H4-4-1C6H11 1.21E+18 -2.84 19903 ! Ref to S3XMCH=P6XC6H10-1E4M PLOG / 0.039 1.21E+18 -2.84 19903 / ! 800 K-2000 K PLOG / 0.197 7.98E+21 -3.70 23365 / ! 800 K-2000 K PLOG / 1.000 2.52E+28 -5.31 28978 / ! 800 K-2000 K PLOG / 10.000 8.05E+37 -7.66 38033 / ! 800 K-2000 K PLOG / 100.000 6.13E+42 -8.70 44718 / ! 800 K-2000 K PLOG / 1.0E+5 1.68E+13 0.21 31241 / ! 800 K-2000 K

C2H5S3XcC6H10 = S6XC8H15-1E 5.23E+18 -2.93 19555 ! Ref to S3XMCH=S6XC7H13-1E PLOG / 0.039 5.23E+18 -2.93 19555 / ! 800 K-2000 K PLOG / 0.197 2.06E+22 -3.73 22876 / ! 800 K-2000 K PLOG / 1.000 3.29E+28 -5.27 28275 / ! 800 K-2000 K PLOG / 10.000 3.31E+37 -7.49 36918 / ! 800 K-2000 K PLOG / 100.000 8.80E+41 -8.42 43157 / ! 800 K-2000 K PLOG / 1.0E+5 2.55E+13 0.17 30061 / ! 800 K-2000 K

C2H5S3XcC6H10=C2H5-4-cC6H9+H 1.19E+16 -2.44 20998 ! Ref to S3XMCH=MCH-3E+H PLOG / 0.039 1.19E+16 -2.44 20998 / ! 800 K-2000 K PLOG / 0.197 5.50E+20 -3.50 24928 / ! 800 K-2000 K PLOG / 1.000 1.93E+28 -5.37 31247 / ! 800 K-2000 K PLOG / 10.000 3.19E+39 -8.14 41683 / ! 800 K-2000 K PLOG / 100.000 1.03E+46 -9.58 49952 / ! 800 K-2000 K PLOG / 1.0E+5 1.87E+12 0.63 34980 / ! 800 K-2000 K

C2H5S3XcC6H10=C2H5-3-cC6H9+H 6.78E+14 -2.23 21396 ! Ref to S3XMCH=MCH-2E+H PLOG / 0.039 6.78E+14 -2.23 21396 / ! 800 K-2000 K PLOG / 0.197 8.10E+19 -3.39 25518 / ! 800 K-2000 K PLOG / 1.000 8.05E+27 -5.38 32106 / ! 800 K-2000 K PLOG / 10.000 6.73E+39 -8.33 43061 / ! 800 K-2000 K PLOG / 100.000 1.12E+47 -9.95 51964 / ! 800 K-2000 K PLOG / 1.0E+5 1.64E+12 0.61 36658 / ! 800 K-2000 K

C2H5S4XcC6H10= PXCH2-5-1C7H13 1.26E+22 -3.85 22627 ! Ref to S4XMCH=P6XC6H10-1E5M PLOG / 0.039 1.26E+22 -3.85 22627 / ! 800 K-2000 K PLOG / 0.197 3.57E+26 -4.89 26638 / ! 800 K-2000 K PLOG / 1.000 2.59E+32 -6.32 32020 / ! 800 K-2000 K PLOG / 10.000 2.07E+41 -8.51 40814 / ! 800 K-2000 K PLOG / 100.000 5.79E+44 -9.15 46530 / ! 800 K-2000 K PLOG / 1.0E+5 3.87E+13 0.20 31782 / ! 800 K-2000 K

C2H5S4XcC6H10=C2H5-4-cC6H9+H 8.38E+20 -3.63 23771 ! Ref to S4XMCH=MCH-3E+H PLOG / 0.039 8.38E+20 -3.63 23771 / ! 800 K-2000 K PLOG / 0.197 8.32E+25 -4.80 28120 / ! 800 K-2000 K PLOG / 1.000 5.73E+32 -6.47 34206 / ! 800 K-2000 K PLOG / 10.000 1.37E+43 -9.02 44242 / ! 800 K-2000 K PLOG / 100.000 7.21E+47 -9.98 51272 / ! 800 K-2000 K PLOG / 1.0E+5 3.78E+12 0.63 34881 / ! 800 K-2000 K

!Ethylcyclohexane reactions

! H abstraction of Ethylcyclohexane

C2H5cC6H11+H = PXC2H4cC6H11+H2 6.66E+06 2.13 8894.8 ! Refer to MCH+H = PXCH2cC6H11+H2 C2H5cC6H11+H = SXC2H4cC6H11+H2 2.55E+05 2.53 4479.0 ! 10LV JetSurF 2.0 C2H5cC6H11+H = C2H5TXcC6H10+H2 4.53E+06 2.11 4098.6 ! Refer to MCH+H = T1XMCH+H2 C2H5cC6H11+H = C2H5S2XcC6H10+H2 2.08E+07 2.10 6474.4 ! Refer to MCH+H = S2XMCH+H2 C2H5cC6H11+H = C2H5S3XcC6H10+H2 2.07E+07 2.12 6441.2 ! Refer to MCH+H = S3XMCH+H2 C2H5cC6H11+H = C2H5S4XcC6H10+H2 1.16E+07 2.11 6339.1 ! Refer to MCH+H = S4XMCH+H2

C2H5cC6H11+CH3 = SXC2H4cC6H11+CH4 7.13E+01 3.25 13556.0 ! 10LV JetSurF 2.0 C2H5cC6H11+CH3 = PXC2H4cC6H11+CH4 3.75E+01 3.27 13516.0 ! Refer to MCH+CH3 = PXCH2cC6H11+CH4 C2H5cC6H11+CH3 = C2H5TXcC6H10+CH4 1.91E+01 3.27 9022.0 ! Refer to MCH+CH3 = T1XMCH+CH4 C2H5cC6H11+CH3 = C2H5S2XcC6H10+CH4 6.68E+01 3.21 11418.0 ! Refer to MCH+CH3 = S2XMCH+CH4 C2H5cC6H11+CH3 = C2H5S3XcC6H10+CH4 7.18E+01 3.26 11303.0 ! Refer to MCH+CH3 = S3XMCH+CH4 C2H5cC6H11+CH3 = C2H5S4XcC6H10+CH4 1.82E+01 3.36 10931.0 ! Refer to MCH+CH3 = S4XMCH+CH4

! isomerization and decomposition of ethylcyclohexane

C2H5cC6H11 = cC6H11+C2H5 1.00 0.00 0.00 ! Ref to MCH = cC6H11+CH3 PLOG / 0.01

1.85E+105 -26.15 129214 / PLOG / 0.0395 1.19E+92 -22.23 122595 / PLOG / 0.197 1.50E+80 -18.67 116938 / PLOG / 0.395 8.65E+63 -13.89 108211 / PLOG / 1 5.93E+64 -14.15 108486 / PLOG / 10 3.59E+45 -8.56 97430 / PLOG / 100 1.66E+33 -4.99 90100 / PLOG / 1.0E+5 1.10E+27 -3.20 86385 /

C2H5cC6H11(+M) = PXCH2cC6H11+CH3(+M) 6.5E+36 -5.84 9.74E+04 ! Ref to C3H8=C2H5+CH3 /2 Matthew A. Oehlschlaeger, PCI 30 1119-1127 LOW / 2.82E+74 -15.74 9.87E+04/ TROE / 0.31 50 3000 9000 / H2/2/ CH4/2/ C2H6/3/ AR/0.7/

! aromatics mechsnism from Yuan et al., Combustion and Flame 162, 3-21; 22-40.

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!! Submechanism of Toluene !!!!!

!————————————— Unimolecular dissociation reactions ———————

A1CH3(+M) = A1CH2+H(+M) 2.78E+15 0.17 9.1168E+04 ! S.J. Klippenstein 2007 PCI LOW/1.00E+98 -22.855 9.9882E+04/ TROE/6.547194E-02 1.511253E+01 9.999996E+09 7.596123E+07/ A1CH3(+M) = A1-+CH3(+M) 1.95E+27 -3.16 1.07447E+05 ! S.J. Klippenstein 2007 PCI LOW/1.00E+98 -22.966 1.2208E+05/ TROE/7.054562E-01 9.999989E+09 4.599180E+02 8.213938E+09/ C6H4CH3+H(+M)=A1 1.00E+14 0.0 0.0 !Refer to A1-+H(+M)=A1(+M) 1997 Wang Frenklach LOW / 6.6E+75 -16.30 7000.0/ TROE/ 1.0 0.1 584.9 6113.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ !————————————— H-Abstraction reactions– A1CH3+H=A1CH2+H2 6.47E+00 3.98 3384.0 !2006 Oehlschlaeger et al. J.Phys.Chem A 110,2006 9867-9873 A1CH3+H=C6H4CH3+H2 3.910e+08 1.800 16352.77 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898 A1CH3+H=A1+CH3 3.90E+08 1.25 2371 !Vasu, Davidson and Hanson 2010, the data is fitted base on the recommendation of Baulch and Ellis ! lead to too much toluene formation !!!C3H3+C4H6=A1CH3+H 3.27E+6 1.28 -4611.0 !Laskin et al. IJCK 32 589-614 2000 6.53E+5 *5 TO interpret the A1CH3 formation in C5H6 flow reactor oxidation !est in this work C3H3+C4H6=A1CH3+H 3.75E+5 1.28 -4611.0 !Laskin et al. IJCK 32 589-614 2000 /2

A1CH3+CH3=A1CH2+CH4 4.220e+14 0.000 22256.21 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898 A1CH3+CH3=C6H4CH3+CH4 1.790E-02 4.460 13637.67 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898 A1CH3+C2H3=A1CH2+C2H4 3.98E+12 0.0 8000.0 !1995 Zhang Mckinnon A1CH3+C3H3=A1CH2+pC3H4 1.6E+12 0.0 15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 A1CH3+C5H5=A1CH2+C5H6 3.2E+12 0.0 17100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 1.6E+12 A1CH3+A1-=A1CH2+A1 2.68e-01 3.95 877.06 !W. K. Metcalfe et al. Energy Fuels 25 (2011) 4915-4936 A1CH3+aC3H5=A1CH2+C3H6 1.6E+12 0.0 15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 A1CH3+iC4H5=A1CH2+C4H6 1.6E+12 0.0 15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 A1CH3+nC4H5=A1CH2+C4H6

1.6E+12 0.0 15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 A1CH3+C6H4CH3=A1CH2+A1CH3 7.9E+13 0.0 12000.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49 nC4H3+pC3H4=¿C6H4CH3 2.40E+10 0.0 0.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190 C6H4CH3=¿nC4H3+pC3H4 4.50E+13 0.0 72500.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190

!** Decomposition of benzyl(A1CH2), fulvenallene(C7H6) and fulvenallenyl(C7H5)

A1CH2=¿C7H6+H 4.47E+129 -32.57 162410.0 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-21318 PLOG / 0.013 4.47E+129 -32.57 162410.0/ PLOG / 0.130 1.29E+123 -30.34 163830.0/ PLOG / 1.000 2.95E+97 -22.95 148280.0/ !close to the experimental measured results of Ronald k. hanson at 1.5 bar PLOG/ 1.500 8.20E+14 0.00E+00 8.07E+04/ PLOG / 10.000 1.26E+39 -6.76 99710.0/ PLOG / 50.000 1.44E+13 0.453 76300/ !HPL

C7H6+H=¿A1CH2 8.80E+8 1.2 -2020 !C. Cavallotti, M. Derudi, R. Rota, PCI 32 (2009) 115-121. A1CH2=o-C6H4+CH3 2.04E+135 -34.08 169130 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-21318 PLOG/ 0.013 2.04E+135 -34.08 169130/ PLOG/ 0.130 6.46E+112 -27.50 155360/ PLOG/ 1.00 5.50E+89 -20.82 141680/ PLOG/ 10.00 5.13E+55 -11.23 116580/ A1CH2+H=A1-+CH3 4.50E+58 -11.9 51860 !S. J. Klippenstein, L. B. Harding, Y. Georgievskii, PC31 (2007) 221-229. PLOG/ 0.0395 4.50E+58 -11.9 51860/ PLOG/ 0.132 2.03E+64 -13.37 59520/ PLOG/ 1.000 5.83E+67 -14.15 68330/ PLOG/ 10.00 8.85E+68 -14.23 78410/

C7H6=cC5H4+C2H2 1.26E+130 -32.19 173970.0 !D. Polino, C. Cavallotti, JPC A 115 (2011) 10281-10289. PLOG / 0.100 2.34E+135 -33.58 179460/ PLOG / 1.000 3.02E+124 -30.18 176460/ PLOG / 10.000 4.27E+129 -31.11 191020/ C7H6=C7H5+H 1.02E+116 -28.46 157860.0 !D. Polino, C. Cavallotti, JPC A 115 (2011) 10281-10289. PLOG / 0.100 1.02E+116 -28.46 157860.0/ PLOG / 1.000 4.90E+66 -14.64 119550.0/ PLOG / 10.000 1.17E+27 -3.54 89150.0/

C5H5+C2H2=¿C7H6+H 1.29E+21 -2.38 32400 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283. PLOG/ 0.0001 1.29E+21 -2.38 32400/ PLOG/ 0.001 3.37E+12 0.22 31060/ PLOG/ 0.01 7.07E+01 3.42 28740/ PLOG/ 0.1 1.58E-01 4.18 29670/ PLOG/ 1.0 6.96E-05 5.17 30930/ PLOG/ 10.0 2.37E-06 5.60 33540/ PLOG/ 100 1.15E-44 17.07 22460/ PLOG/ 1000 8.31E-37 14.56 29740/

C7H6+H=¿C5H5+C2H2 6.81E+24 -3.04 14950 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283. PLOG/ 0.0001 6.81E+24 -3.04 14950/ PLOG/ 0.001 6.87E+16 -0.62 13700/ PLOG/ 0.01 5.39E+06 2.41 11550/ PLOG/ 0.1 3.65E+01 3.93 11460/ PLOG/ 1.0 1.22E-06 6.15 11040/ PLOG/ 10.0 2.65E-15 8.75 10810/ PLOG/ 100 8.55E-21 10.35 12590/ PLOG/ 1000 2.05E-30 13.09 13020/ C7H6+H=C7H5+H2 1.90E+08 1.847 4965.0 !G. da

Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048. C7H6+CH3=C7H5+CH4 1.87E+04 2.724 6008.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.

C7H5=C4H2+C3H3 8.71E+92 -23.08 117070.0 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-21318 PLOG / 0.013 8.71E+92 -23.08 117070.0/ PLOG / 0.130 1.82E+102 -25.22 130330.0/ PLOG / 1.000 8.51E+82 -19.18 125340.0/ PLOG / 10.000 2.40E+56 -11.65 106750.0/ nC4H3+C3H3=C7H6 1.00E+13 0.00 0.0 !Y. Sakai et al. PCI32 (2009) 411-418 C7H5=C5H3+C2H2 3.16E+83 -20.81 109410.0 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-21318 PLOG / 0.013 3.16E+83 -20.81 109410.0/ PLOG / 0.130 7.59E+102 -25.66 132390.0/ PLOG / 1.000 2.82E+90 -21.38 135620.0/ PLOG / 10.000 4.37E+90 -21.04 143990.0/ C6H4CH3=A1CH2 3.09E+73 -18.22 69670 !Enoch Dames Hai Wang 2013 PCI34 PLOG/ 0.1 3.09E+73 -18.22 69670/ PLOG/ 1.0 2.91E+59 -13.86 64518/ PLOG/ 10.0 6.76E+40 -8.54 54069/ PLOG/ 50.0 3.66E+26 -3.98 49795/ C6H4CH3+H=A1CH2+H 1.0E+13 0.0 0.0 !Bounaceur et al 2005 C6H4CH3=o-C6H4+CH3 6.11E+45 -8.857 94350.6 !1997 Madden et al. RRKM A1-=o-C6H4+H PLOG / 0.500 6.11E+45 -8.857 94350.6/ PLOG / 1.000 8.00E+41 -7.72 92300.3/ PLOG / 10.000 1.66E+30 -4.318 85756.9/ A1CH2=C5H5+C2H2 4.08E+134 -34.08 169130 !EST this work 5 times slower than the reaction A1CH2=o-C6H4+ch3 PLOG/ 0.013 4.08E+134 -34.08 169130/ PLOG/ 0.130 1.29E+112 -27.50 155360/ PLOG/ 1.00 1.10E+89 -20.82 141680/ PLOG/ 10.00 1.03E+55 -11.23 116580/ PLOG/ 50.000 1.44E+13 0.453 76300/

!* Reactions of benzene(A1) and fulvene ********* A1-+H(+M)=A1(+M) 1.00E+14 0.0 0.0 !1997 Wang Frenklach RRKM LOW / 6.6E+75 -16.30 7000.0/ TROE/ 1.0 0.1 584.9 6113.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/

!——— A1+H=A1-+H2 2.50E+14 0.0 16000.0 !Emdee et al.J. Phys. Chem. 1992, 96, 2151-2161 A1-+CH4=A1+CH3 3.89E-03 4.6 5256.0 !1999 Tokmakov et al. A1-+C2H6=A1+C2H5 2.10E+11 0.0 4443.0 !2001 Park et al. C5H6+A1-=C5H5+A1 3.10E+11 0.0 5500.0 !2001 Backskay Mackie nC4H3+C2H3=A1 2.87E+14 0.0 817.0 !1988 Duran et al. Fit data in 2005 Sivaramakrishnan et al. C3H3+aC3H5=fulvene+2H 3.26E+29 -5.4 3390.0 !MillerKlippenstein 2003. aC3H4+C3H2=A1 7.40E+12 -0.7 920.0 !2002 D'Anna et al. pC3H4+C3H2=A1 1.40E+13 -0.8 1030.0 !2002 D'Anna et al. aC3H4+C3H3=A1+H 2.20E+11 0.0 2000.0 !2002 D'Anna et al. C4H4+C2H3=A1+H 1.90E+12 0.0 2510.0 !1997 LindstedtSkevis pC3H4+C3H3=A1+H 2.20E+11 0.0 2000.0 !1987 WuKern C4H4+C2H2=A1 4.47E+11 0.0 30010.0 !1986 ChanmugathasHeicklen C2H2+nC4H5=H+A1 1.37E16 -1.00 8896 !MillerKlippenstein 2003 PLOG /0.01 1.37E16 -1.00 8896./ PLOG /0.025 2.94E16 -1.09 9259./ PLOG /0.1 1.37E16 -1.00 8898./ PLOG /1. 1.385E16 -1.00 8900./ PLOG /10. 1.69E16 -1.03 8967./ PLOG /100. 1.65E16 -1.01 9480./ C2H2+nC4H5=H+fulvene 1.52E15 -0.76 8767 !MillerKlippenstein 2003 PLOG /0.01 1.52E15 -0.76 8767./ PLOG /0.025

1.52E15 -0.76 8767./ PLOG /0.1 1.52E15 -0.76 8769./ PLOG /1. 4.63E15 -0.89 9142./ PLOG /10. 1.74E19 -1.86 12383./ PLOG /100. 1.23E20 -2.00 16152./ !MillerKlippenstein 2003 C2H2+iC4H5=H+A1 1.47E+23 -3.28 24907 !MillerKlippenstein 2003 PLOG /0.01 1.47E+23 -3.28 24907./ PLOG /0.025 1.47E+23 -3.28 24907./ PLOG /0.1 1.47E+23 -3.28 24907./ PLOG /1. 1.67E+23 -3.30 24959./ PLOG /10. 8.25E+24 -3.76 24562./ PLOG /100. 5.37E+32 -5.84 35023./ C2H2+iC4H5=H+fulvene 6.50E+24 -3.44 20319. !MillerKlippenstein 2003 PLOG /0.01 6.50E+24 -3.44 20319./ PLOG /0.025 1.01E+34 -5.94 28786./ PLOG /0.1 6.50E+24 -3.44 20319./ PLOG /1. 6.80E+24 -3.45 20337./ PLOG /10. 9.70E+25 -3.76 21326./ PLOG /100. 5.22E+41 -7.94 39597./ nC4H5+C2H3=A1+H2 1.84E-13 7.1 -3611.0 !1989 Westmoreland et al. C3H3+C3H3=fulvene 6.3069E+76 -19.07 31542. !MillerKlippenstein 2003 PLOG /0.03947 6.3069E+76 -19.07 31542./ PLOG /1. 1.3798E+66 -15.66 28260./ PLOG /10. 1.2584E+56 -12.61 23515./ C3H3+C3H3=A1 1.8189E+74 -18.14 31896. !MillerKlippenstein 2003 PLOG /0.03947 1.8189E+74 -18.14 31896./ PLOG /1. 3.1609E+55 -12.55 22264./ PLOG /10. 3.8888E+50 -11.01 20320./ fulvene=A1 5.62E+81 -19.36 121500.0 !2003 MillerKlippenstein 2003 PLOG / 0.0395 5.62E+81 -19.36 121500.0/ PLOG / 1.0000 1.45E+45 -8.90 96999.0/ PLOG / 10.0000 2.95E+31 -4.97 88465.0/ C3H3+C3H3=A1-+H 1.0467E+54 -11.88 28757. !2003 MillerKlippenstein 2003 PLOG /0.03947 1.0467E+54 -11.88 28757./ PLOG /1. 1.6975E+48 -9.977 36755./ PLOG /10. 3.6712E+26 -3.879 28963./ fulvene+H=A1+H 4.94E+18 -1.28 5411 !Ahren W. Jasper 2013 PLOG/ 0.00132 4.94E+18 -1.28 5411/ PLOG/ 0.0132 2.15E+22 -2.28 8429/ PLOG/ 0.132 5.60E+26 -3.47 12818/ PLOG/ 1.000 1.66E+25 -2.99 13691/ PLOG/ 1.312 5.06E+25 -3.12 14226/ PLOG/ 13.12 2.20E+27 -3.48 19199/ fulvene=A1-+H 2.57E+97 -23.2 153470.0 !2003 MillerKlippenstein 2003 PLOG / 0.0395 2.57E+97 -23.2 153470.0/ PLOG / 1.0000 2.24E+68 -14.7 142570.0/ PLOG / 10.0000 8.51E+24 -2.5 113330.0/ A1-(+M)=o-C6H4+H(+M) 4.300E+12 0.616 77313. !RRKM 00-HAI-FRE LOW/ 1.000E+84 -18.866 90064/ !20130218 TROE/ 0.902 696. 358. 3856. / H2/2.0/ CH4/2.0/

n-C6H5 = A1- 3.70E+63 -16.49 36100. !1997WangFrenklach RRKM PLOG/ 0.013 3.70E+63 -16.49 36100./ PLOG/ 0.026 1.30E+62 -15.94 35800./ PLOG/ 0.118 1.30E+59 -14.78 35600./ PLOG/ 1.00 5.10E+54 -13.11 35700./ PLOG/ 10.00 3.50E+46 -10.44 33600./ n-C6H5 = o-C6H4 + H 1.60E+65 -16.00 58400. !1997WangFrenklach RRKM PLOG/ 0.013 1.60E+65 -16.00 58400./ PLOG/ 0.026 2.70E+65 -15.93 59700./ PLOG/ 0.118 1.50E+64 -15.32 61500./ PLOG/ 1.00 1.30E+59 -13.56 62000./ PLOG/ 10.00 1.10E+50 -10.69 60900./ n-C6H5+H = C4H4+C2H2 1.60E+19 -1.60 2220.0 !1997WangFrenklach RRKM PLOG/ 0.026 1.60E+19 -1.60 2220.0/ PLOG/ 0.118 1.30E+20 -1.85 2960.0/ PLOG/ 1.00 6.30E+25 -3.34 10014.0/ A1-=nC4H3+C2H2 3.55E+78 -17.787 137467.2 !1997 Madden et al. RRKM PLOG / 0.500 3.55E+78 -17.787 137467.2/ PLOG / 1.000 3.92E+74 -16.6 135581.1/ PLOG / 10.000 1.79E+61 -12.663 128678.3/ nC4H3+C2H2=o-C6H4+H 1.90E+36 -7.21 17900.0 !1994 WangFrenklach RRKM PLOG / 0.0132 9.20E+33 -6.57

15900.0/ PLOG / 0.0263 1.90E+36 -7.21 17900.0/ PLOG / 0.1184 3.50E+41 -8.63 23000.0/ PLOG / 1.0000 6.90E+46 -10.01 30100.0/ PLOG / 10.0000 3.10E+49 -10.59 37700.0/ A1-+H=o-C6H4+H2 2.36E-06 5.80 11714 !2001 A. M. Mebel and M.C.Lin PLOG/ 0.132 2.36E-06 5.80 11714/ PLOG/ 1.000 1.16E-14 8.13 8766/ PLOG/ 10.00 2.58E-22 10.22 5350/ l-C6H4+H=A1- 4.00E+77 -19.99 28100.0 !1994 WangFrenklach RRKM plog / 0.0132 4.40E+74 -19.09 25800.0/ plog / 0.0263 4.00E+77 -19.99 28100.0/ plog / 0.1184 4.70E+78 -20.10 29500.0/ plog / 1.0000 1.70E+78 -19.72 31400.0/ plog / 10.0000 3.90E+69 -16.63 34100.0/

Reactions of cC5H5-13E5M(Methylcyclopentadiene

C5H5+CH3=¿cC5H5-13E5M 9.10E+109 -29.19 41906 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 9.10E+109 -29.19 41906/ PLOG/ 1.00 3.06E+105 -27.05 47952/ PLOG/ 10.0 2.38E+94 -23.52 45184/ PLOG/ 100 1.09E+70 -16.33 32296/ C5H5+CH3=¿fulvene+H2 9.25E+01 2.19 8815 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 9.25E+01 2.19 8815 / PLOG/ 1.00 1.14E+15 -1.40 20266 / PLOG/ 10.0 3.62E+31 -5.90 35631 / PLOG/ 100 3.38E+43 -9.05 49742 / cC5H5-13E5M=¿C5H5+CH3 4.49E+77 -19.26 89496 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 4.49E+77 -19.26 89496/ PLOG/ 1.00 2.01E+89 -21.78 105380/ PLOG/ 10.0 6.89E+84 -20.17 106554/ PLOG/ 100 4.46E+71 -16.16 100961/ cC5H5-13E5M=¿fulvene+H2 3.38E+77 -21.53 96791 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 3.38E+77 -21.53 96791/ PLOG/ 1.00 2.04E+94 -25.05 118602/ PLOG/ 10.0 1.05E+97 -25.23 126838/ PLOG/ 100 3.85E+84 -21.21 124346/ C5H5+CH3=¿C5H5CH2-2+H 7.49E+13 -0.30 11640 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 7.49E+13 -0.30 11640/ PLOG/ 1.00 7.93E+27 -4.14 24060/ PLOG/ 10.0 7.18E+44 -8.75 40084/ PLOG/ 100 1.31E+53 -10.86 51760/ C5H5+CH3=¿C5H5CH2-3+H 2.18E+14 -0.40 17024 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 2.18E+14 -0.40 17024/ PLOG/ 1.00 1.31E+23 -2.81 24726/ PLOG/ 10.0 6.08E+38 -7.08 39076/ PLOG/ 100 1.81E+52 -10.67 54105/ C5H5+CH3=¿C5H5CH2-1+H 8.13E+25 -3.51 41018 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 8.13E+25 -3.51 41018/ PLOG/ 1.00 3.83E+26 -3.69 41579/ PLOG/ 10.0 1.16E+33 -5.47 47110/ PLOG/ 100 1.03E+48 -9.54 61181/ cC5H5-13E5M=¿C5H5CH2-2+H 1.38E+96 -24.49 116744 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 1.00 1.38E+96 -24.49 116744/ PLOG/ 10.0 1.54E+98 -24.53 124128/ PLOG/ 100 3.13E+86 -20.76 121667/ cC5H5-13E5M=¿C5H5CH2-3+H 1.61E+100 -25.89 121934 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 1.00 1.61E+100 -25.89 121934/ PLOG/ 10.0 2.05E+103 -26.14 130620/ PLOG/ 100 7.82E+93 -22.94 130454/ cC5H5-13E5M=¿C5H5CH2-1+H 9.33E+109 -29.66 135070 !Sandeep

Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 1.00 9.33E+109 -29.66 135070/ PLOG/ 10.0 1.07E+116 -30.36 147389/ PLOG/ 100 1.21E+114 -28.95 154902/ C5H5CH2-2=fulvene+H 1.35e+58 -13.11 73890 !Polimi V2012 C5H5CH2-2=A1+H 9.25e+43 -9.19115 55756.8 !Polimi V2012 cC5H5-13E5M+H=C5H5CH2-2+H2 1.30e+06 2.38 2800.00 !Polimi V2012 C5H5CH2-1=C5H5CH2-2 1.69e+30 -5.9432 21537.5 !Polimi V2012 C5H5CH2-2=C5H5CH2-3 1.08e+41 -8.73397 44399 !Polimi V2012 C5H5CH2-3=fulvene+H 3.67e+43 -9.19 57330 !Polimi V2012 C5H5CH2-1=C5H5CH2-3 9.23e+27 -5.12362 28314.7 !Polimi V2012 C5H5CH2-3=A1+H 1.38e+46 -9.72349 57338 !Polimi V2012 C5H5CH2-1=fulvene+H 1.07e+29 -5.32 32810 !Polimi V2012 C5H5CH2-1=A1+H 1.98e+31 -6.06562 20629.6 !Polimi V2012

H+cC5H5-13E5M=¿CH3+C5H6 1.500E+13 0.0 2000.0 !Polimi V2012

CH3+cC5H5-13E5M=¿CH4+A1+H 3.903E+05 2.0 3544.16 !Polimi V2012 C2H5+cC5H5-13E5M=¿C2H6+A1-
2.298E+05 2.0 6224.33 !Polimi V2012

C5H5+CH3=¿cC5H5-13E1M 9.10E+109 -29.19 41906 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 9.10E+109 -29.19 41906/ PLOG/ 1.00 3.06E+105 -27.05 47952/ PLOG/ 10.0 2.38E+94 -23.52 45184/ PLOG/ 100 1.09E+70 -16.33 32296/

cC5H5-13E1M=¿C5H5+CH3 4.49E+77 -19.26 89496 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882 PLOG/ 0.01 4.49E+77 -19.26 89496/ PLOG/ 1.00 2.01E+89 -21.78 105380/ PLOG/ 10.0 6.89E+84 -20.17 106554/ PLOG/ 100 4.46E+71 -16.16 100961/

H+cC5H5-13E1M=¿CH3+C5H6 1.500E+13 0.0 2000.0 !Polimi V2012

Reactions of C5H5(1,3-Cyclopentadienyl) and C5H6(1,3-cyclopentadiene)

C3H3+C2H2=¿C5H5 6.17E+66 -15.7 47729 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 6.17E+66 -15.7 47729/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 6.87E+55 -12.5 42000/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 1.13E+43 -8.80 34983/ !L. V. Moskaleva, M. C. Lin 1999 C5H5=¿C3H3+C2H2 2.79E+79 -18.3 130768 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 2.79E+79 -18.3 130768/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 1.98E+68 -15.0 124824/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 5.70E+54 -11.10 116874/ !L. V. Moskaleva, M. C. Lin 1999 C5H5=IC5H5 2.25E+108 -28.2 127755 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 2.25E+108 -28.2 127755/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 1.21E+109 -28.1 130355/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 2.08E+112 -28.6 136922/ !L. V. Moskaleva, M. C. Lin 1999 C5H5=C5H52 5.17E+80 -20.4 96136 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 5.17E+80 -20.4 96136/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 5.92E+78 -19.5 96640/ !L.

V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 1.32E+78 -19.0 99133/ !L. V. Moskaleva, M. C. Lin 1999 C3H3+C2H2=¿lC5H5 6.87E+71 -18.2 45334 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 6.87E+71 -18.2 45334/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 4.11E+72 -18.2 45411/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 1.55E+77 -19.1 49598/ !L. V. Moskaleva, M. C. Lin 1999 lC5H5=¿C3H3+C2H2 3.12E+82 -20.6 68862 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 3.12E+82 -20.6 68862/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 1.95E+83 -20.6 68951/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 5.61E+87 -21.5 73148/ !L. V. Moskaleva, M. C. Lin 1999 C3H3+C2H2=¿C5H52 1.34E+68 -16.9 51542 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 1.34E+68 -16.9 51542/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 2.70E+53 -12.6 41445/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 1.81E+35 -7.6 76409/ !L. V. Moskaleva, M. C. Lin 1999 C5H52=¿C3H3+C2H2 3.40E+80 -19.2 102213 !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 0.132 3.40E+80 -19.2 102213/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 1.000 7.48E+65 -15.0 92200/ !L. V. Moskaleva, M. C. Lin 1999 PLOG/ 10.00 4.57E+47 -9.9 51542/ !L. V. Moskaleva, M. C. Lin 1999 C5H5+H(+M)=C5H6(+M) 1.000E+14 0.000 0.00 !92-EMD-BRE, est., 94-FRA-HER LOW / 4.400E+80 -18.280 12994.0/ !96-DAV-WAN, 97-WAN-FRE TROE / 0.068 400.7 4135.8 5501.9 / H2/2.0/ CH4/2.0/ C5H6(+M)= aC3H4+C2H2(+M) 3.8E+17 0.0 1.04E+05 !Mackie et al. 2001 PCCP LOW /1.00E+98 -22.25 126321.5/ TROE /1.440547E-01 5.357622E+00 3.283766E+03 6.710101E+09/ H2 /2.0/ CH4 /2.0/ C5H6+H=C5H5+H2 7.2E+13 0 3500.0 !Better for C5H6 flow reactor pyrolysis C5H6+H=C2H2+aC3H5 7.74E+36 -6.2 32890.0 !zhong bozzeli j phys chem a 102 ! sensitive reaction better for C5H6 flow reactor pyrolysis C5H6+C2H3=C5H5+C2H4 6.00E+12 0.0 0.0 !2001 BacskayMackie 6.00E+12 C5H6+CH3=C5H5+CH4 0.18 4.0 0.0 !zhong bozzeli j phys chem a 102: 3537 1998 aC3H5+C2H2=lC5H7 3.0e+11 0.0 6883.4 !ziegler et al. j. anal.apply.pyrolysis 73 212-230 (2005) C5H6+H=lC5H7 2.4e+73 -17.85 31500.0 ! lC5H5+H=C5H4+H2 1.81E+12 0.0 0.0 !1986 TsangHampson C2H5+H in 2002 RichterHoward lC5H5+CH3=C5H4+CH4 1.95E+13 -0.50 0.0 !1986 TsangHampson C2H5+CH3 in 2002 RichterHoward aC3H5+C2H3=lC5H7+H 1.00E+13 0.0 0.0 !USC Mech II Est. C5H5+aC3H4=A1+C2H3 2E+10 0 0 !EST C5H5+pC3H4=A1+C2H3 2E+10 0 0 !EST C4H5-2+C2H4=C5H6+CH3 5.00E+14 0.0 25000.0 ! USC Mech V2.0

mechanism for cyclopentadiene decomposition

C5H6+C5H5=¿C9H8+CH3 1.574E+25 -3.935 23108 !Carlo Cavallotti 2012 JPCA C5H6+C5H5=¿A1+nC4H5 7.430E+29 -4.515 40873 !Carlo Cavallotti 2012 JPCA CH3+nC4H3=¿C5H6 1.000E+13 0.0 0.0 !Polimi V2012 C3H3+C2H4=H+C5H6 5.000E+10 0.0 20400.0 !Polimi V2012 CH3+C4H2=¿C5H5 1.000E+11 0.0 7600.0 !Polimi V2012 CH3+C5H5=nC4H5+C2H3 1.000E+12 0.0 3000.0 !Polimi V2012 CH3+C5H5=¿C4H6+C2H2 1.500E+12 0.0 3000.0 !Polimi V2012 C2H3+aC3H4=¿C5H6+H 5.000E+11 0.0 3000.0 !Polimi V2012 C2H3+pC3H4=¿C5H6+H 5.000E+11 0.0 3000.0 !Polimi V2012 C5H5+C5H6=¿A1C2H3+C2H3 3.000E+55 -11.390 66311.0 !Polimi V2012 C5H5+C5H6=¿C9H7+CH4

5.000E+01 3.100 14800.0 !Polimi V2012 C5H5+C5H6=¿0.5A1+0.5nC4H5+0.5A1C2H3+0.5C2H3 5.250E+16 -1.407 23454.0 !Polimi V2012 C5H5+C5H6=¿A1CH2+0.5aC3H4+0.5pC3H4 1.000E+12 .000 25000.0 !Polimi V2012 aC3H5+C5H6=¿C3H6+C5H5 2.407E+05 2.0 15253.34 !Polimi V2012 nC4H5+C5H6=¿aC3H5+A1 1.000E+12 0.00 5000.0 !Polimi V2012

!Reactions of C6H4

o-C6H4=C4H2+C2H2 6.50E+13 0.0 83000.0 !1999 Moskaleva et al. RRKM PLOG / 0.1315 1.95E+90 -21.3 139396.2/ PLOG / 1.0000 2.07E+85 -19.6 138901.4/ PLOG/ 5.000 7.89E+75 -16.8 134903.4/ PLOG / 10.0000 7.89E+75 -16.8 134903.4/ l-C6H4 + H = o-C6H4+ H 8.70E+45 -9.61 22300. !1997 WangFrenklach PLOG/ 0.013 8.70E+45 -9.61 22300./ PLOG/ 0.026 2.20E+47 -9.98 24000./ PLOG/ 0.118 9.70E+48 -10.37 27000./ PLOG/ 1.000 1.40E+54 -11.70 34500./ PLOG/ 10.00 5.70E+55 -11.98 41900./ l-C6H4+H=C6H3+H2 1.33E+06 2.5 9240.0 !USC Mech II C3H2+C3H2=l-C6H4 3.00E+11 0.0 0.0 !1987 WuKern C3H3+C3H3=A1 C4H2+C2H2=l-C6H4 4.47E+11 0.0 30010.0 !1986 ChanmugathasHeicklen C4H4+C2H2=A1 in 2002 RichterHoward nC4H3+C2H2=l-C6H4+H 3.70E+16 -1.2 11100.0 !1997 WangFrenklach RRKM 20Torr C4H4+C2H=l-C6H4+H 1.20E+13 0.0 0.0 !USC Mech II C6H3+H=l-C6H4 4.20E+44 -10.27 7890.0 !1WangFrenklach RRKM iC4H3+H=C4H4 in 1997 PLOG / 0.0263 4.20E+44 -10.27 7890.0/ PLOG / 0.1184 5.30E+46 -10.68 9270.0/ PLOG / 1.0000 3.40E+43 -9.01 12120.0/ C4H2+C2H=C6H3 1.10E+30 -6.30 2790.0 !1997 WangFrenklach RRKM PLOG / 0.0263 1.10E+30 -6.30 2790.0/ PLOG / 0.1184 1.30E+30 -6.12 2510.0/ PLOG / 1.0000 4.50E+37 -7.68 7100.0/ C6H2+H=C6H3 4.30E+45 -10.15 13250.0 !1997 WangFrenklach RRKM C4H2+H=iC4H3 in 1997 h PLOG / 0.0263 4.30E+45 -10.15 13250.0/ PLOG / 0.1184 2.60E+46 -10.15 15500.0/ PLOG / 1.0000 1.10E+30 -4.92 10800.0/ C6H3+H=C4H2+C2H2 2.40E+19 -1.6 2800.0 !1997 WangFrenklach RRKM 20Torr iC4H3+H=C2H2+C2H2 in 1997 WangFrenklach o-C6H4+C3H3=¿C7H5+C2H2 6.93E+59 -12.732 53252 !Akira Matsugi and Akira Niyoshi 2012 PCCP,14. PLOG/ 0.0132 6.93E+59 -12.732 53252/ PLOG/ 0.132 4.36E+61 -13.054 61485/ PLOG/ 1.000 9.61E+54 -11.098 61937/ PLOG/ 10.00 2.58E+38 -6.427 55219/ PLOG/ 100.0 3.29E+15 -0.001 45393/ C7H5+C2H2=¿o-C6H4+C3H3 4.68E+61 -13.236 79195 !Akira Matsugi and Akira Niyoshi 2012 PCCP,14. PLOG/ 0.0132 4.68E+61 -13.236 79195/ PLOG/ 0.132 2.76E+63 -13.551 87406/ PLOG/ 1.000 5.74E+56 -11.587 87838/ PLOG/ 10.00 1.44E+40 -6.908 81096/ PLOG/ 100.0 1.81E+17 -0.480 71271/ o-C6H4+C3H3=¿C9H7 7.46E+100 -25.035 61535.403 !Akira Matsugi and Akira Niyoshi 2012 PCCP,14. 20130823 PLOG/ 0.0132 1.49E+100 -25.035 61535.403/ !/5 PLOG/ 0.132 1.12E+79 -18.907 49031.8081 / !/5 PLOG/ 1.000 7.14E+57 -12.867 34883.772 / !/5 PLOG/ 10.00 1.12E+37 -6.994 20138.245 / !/5 PLOG/ 100.0 6.12E+24 -3.553 11067.3913 / !/5 C9H7=¿o-C6H4+C3H3 5.46E+121 -29.395 199434.5939 PLOG/ 0.0132 8.44E+108 -29.395 199434.5939 / PLOG/ 0.132 4.77E+92 -25.566 193628.3812 / PLOG/ 1.000 9.17E+71 -20.893 183479.1826 / PLOG/ 10.00 3.91E+54 -15.042 168832.8069 / PLOG/ 100.0

2.35E+78 -10.189 155667.9384 /

reactions of C5H2 C5H3 cC5H4(cyclopentadienylidene)C5H4

C4H2+CH2*=C5H3+H 1.30E+13 0.0 0.0 !1992 MillerMelius C4H2+CH2=C5H3+H 3.00E+13 0.0 0.0 !1992 MillerMelius C4H2+CH=C5H2+H 1.00E+14 0.0 0.0 !1992 MillerMelius C5H3+H=C5H2+H2 6.03E+13 0.0 15103.0 !1992 Baulch et al. CH3+H=CH2+H2 in 2002 RichterHoward C5H3+CH3=A1 4.3E+12 0.0 0.0 !Estimated C5H3+CH=C6H2+H+H 5.00E+13 0.0 0.0 ! Estimated C5H3+CH2=l-C6H4+H 5.00E+13 0.0 0.0 ! = C3H3+CH2 cC5H4=C5H4 1.98E+12 0.56 42240.0 PLOG / 0.1 2.30E+39 -8.81 47800.0 / != cC3H4 = aC3H4 99DAV/LAW RRKM PLOG / 0.4 7.59E+40 -9.07 48831.0 / PLOG / 1 4.89E+41 -9.17 49594.0 / PLOG / 2 8.81E+41 -9.15 50073.0 / PLOG / 5 4.33E+41 -8.93 50475.0 / PLOG / 10 7.20E+40 -8.60 50600.0 / PLOG / 100 1.60E+35 -6.64 49500.0 / cC5H4+H=¿C5H5 6.61E+12 0.3 770 ! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP 2011,13 C5H5=¿cC5H4+H 5.37E+17 -0.55 115500 ! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP 2011,13 cC5H4+A1CH3=C5H5+A1CH2 4.47E+03 2.37 3300 ! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP 2011,13 C4H2+CH3=C5H4+H 2.40E+09 0.91 20700.0 !1999 Davis et al. C2H2+CH3=aC3H4+H in 2010 Li(Ph.D. Thesis) C4H+CH4=C5H4+H 2.40E+09 0.91 20700.0 !1999 Davis et al. C2H2+CH3=aC3H4+H in 2010 Li(Ph.D. Thesis) aC3H4+C2H=C5H4+H 9.60E+13 0.0 0.0 !2000 Appel et al. C2H2+C2H=C4H2+H in 2010 Li(Ph.D. Thesis) C5H3+H=C5H4 3.6308E+36 -7.36 6039. !2008 Miller Senosiain Klippenstein C3H3+H=pC3H4 20130821 PLOG /0.03947 7.26E+36 -7.36 6039./ !*2 PLOG /1. 1.59E+30 -5.06 4861./ !*2 PLOG /10. 2.14E+24 -3.15 3261./ !*2 C5H4+H=C5H3+H2 1.00E+06 2.50 5000.0 !Alzueta et al. 1998

C4H+H(+M) = C4H2(+M) 1.000E+17 -1.000 0.00 != C2H +H LOW / 3.750E+33 -4.800 1900.00 / TROE/ 0.6464 132.00 1315.00 5566.0 / C4H+H2 = H+C4H2 4.90E+05 2.500 560.00 C4H2+C2H=C6H2+H 9.60E+13 0.0 0. != C2H2 + C2H HACA C2H2+C4H=C6H2+H 7.80E+13 0.0 0. != C2H2 + C2H C4H+C2H=C6H2 5.00E+13 0.0 0.0 != C2H+C2H C3H2+C3H2=C6H2+H2 1.00E+13 0.0 0.0 !MODIF !C6H2+C2H=C8H2+H 9.60E+13 0.0 0. != C2H2 + C2H HACA

A1C2H-=C6H3C2H+H 6.11E+45 -8.857 94350.6 !1997 Madden et al. RRKM A1-=o-C6H4+H plog / 0.500 6.11E+45 -8.857 94350.6/ plog / 1.000 8.00E+41 -7.72 92300.3/ plog / 10.000 1.66E+30 -4.318 85756.9/ A1C2H-=C6H3+C2H2 3.55E+78 -17.787 137467.2 !1997 Madden et al. RRKM A1-=nC4H3+C2H2 plog / 0.500 3.55E+78 -17.787 137467.2/ plog / 1.000 3.92E+74 -16.6 135581.1/ plog / 10.000 1.79E+61 -12.663 128678.3/ A1C2H-+H=C6H3C2H+H2 4.40E-13 7.831 9261.0 !2001 Mebel et al. A1-+H=o-C6H4+H2 A1C2H-=nC4H3+C4H2 3.55E+78 -17.787 137467.2 !1997 Madden et al. RRKM A1-=nC4H3+C2H2 plog / 0.500 3.55E+78 -17.787 137467.2/ plog / 1.000 3.92E+74 -16.6 135581.1/ plog / 10.000 1.79E+61 -12.663 128678.3/

C6H3C2H=C4H2+C4H2 1.95E+90 -21.3 139396.2 !refer to 1999 Moskaleva et al. o-C6H4=C4H2+C2H2 PLOG / 0.1315 1.95E+90 -21.3 139396.2/ PLOG / 1.0000 2.07E+85 -19.6 138901.4/ PLOG/ 5.000 7.89E+75 -16.8 134903.4/ PLOG / 10.0000 7.89E+75 -16.8 134903.4/

A1C2H-+H(+M)=A1C2H(+M) 1.00E+14 0.0 0.0 !1997 WangFrenklach A1-+H(+M)=A1(+M) in 1997 WangFrenklach LOW / 6.60E+75 -16.30 7000.0/ TROE/ 1.0 0.1 584.9 6113.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ ! shield in this work, the estimation to toluene is not adeqate. !A1C2H(+m)=A1-+C2H(+m) 7.80e+27 -3.16 1.07447e+05 !estimated from Klippenstein 2007 ! LOW/4.00E+98 -22.966 1.2208E+05/ ! TROE/7.054562E-01 9.999989E+09 4.599180E+02 8.213938E+09/ A1C2H(+M)=A1CC+H 2.78E+15 0.17 9.1168E+04 !estimated from 2007 Kliphenstein et al. A1CH3(+M) = A1CH2+H(+M) LOW/1.00E+98 -22.855 9.9882E+04/ TROE/6.547194E-02 1.511253E+01 9.999996E+09 7.596123E+07/ A1C2H+H=A1cC2H2+H 2.30E+15 -0.26 7600.0 !1999 Davis et al. pC3H4+H=aC3H4+H 0.1atm A1+C2H=A1C2H+H 5.00E+13 0.0 0.0 !1997 WangFrenklach A1C2H+H=A1CC+H2 2.50E+14 0.0 16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in 1997 WangFrenklach A1C2H+H=A1C2H-+H2 1.084e17 -0.70 20011.2 !ref A1+H=A1-+H2 *5/6 A1-+C2H2=A1C2H+H 2.66E+32 -5.3 23786.9 !I.V. Tokmakov, M.C. Lin, J. Am. Chem. Soc. 125(2003) 11397-11408. A1-+C4H4=A1C2H+C2H3 3.20E+11 0.0 1350.0 !1988 Harris et al. nC4H5+C4H2=A1C2H+H 3.16E+11 0.0 1800.0 !1984 Cole et al.

A1-+C2H3=A1CCH2+H 1.80E+31 -4.63 31652. !1997 WangFrenklach RRKM PLOG/ 0.026 1.80E+31 -4.63 31652./ PLOG/ 0.118 5.80E+18 -1.00 26852./ PLOG/ 1.000 8.50E-02 4.71 18424./ A1-+C2H3=A1CHCH+H 1.50E+32 -4.91 35504. !1997 WangFrenklach RRKM PLOG/ 0.026 1.50E+32 -4.91 35504./ PLOG/ 0.118 5.10E+20 -1.56 31412./ PLOG/ 1.000 9.40E+00 4.14 23234./ A1CHCH+H=A1CCH2+H 2.30E+37 -6.00 35164. !1997 WangFrenklach RRKM PLOG/ 0.026 2.30E+37 -6.00 35164./ PLOG/ 0.118 1.20E+25 -2.42 30530./ PLOG/ 1.000 9.90E+04 3.37 22040./ A1-+C2H2=A1CHCH 7.70E+40 -9.19 13400.0 !1994 WangFrenklach RRKM plog / 0.0132 4.00E+39 -8.94 12000.0/ plog / 0.0263 7.70E+40 -9.19 13400.0/ plog / 0.1184 9.90E+41 -9.26 15700.0/ plog / 1.0000 7.00E+38 -8.02 16400.0/ plog / 10.0000 7.90E+29 -5.15 13700.0/ A1C2H+H=A1CHCH 1.00E+54 -12.76 17185.0 !1997 WangFrenklach RRKM plog / 0.0263 1.00E+54 -12.76 17185.0/ plog / 0.1184 1.20E+51 -11.69 17300.0/ plog / 1.0000 3.00E+43 -9.22 15300.0/ A1C2H+H=A1CCH2 1.00E+54 -12.76 17185.0 !1997 WangFrenklach RRKM A1C2H+H=A1CCH2 in 1997 WangFrenklach plog / 0.0263 1.00E+54 -12.76 17185.0/ plog / 0.1184 1.20E+51 -11.69 17300.0/ plog / 1.0000 3.00E+43 -9.22 15300.0/ A1CHCH+H=A1C2H+H2 3.00E+13 0.0 0.0 !GRI C2H3+H=C2H2+H2in 1997 WangFrenklach A1CCH2+H=A1C2H+H2 3.00E+13 0.0 0.0 !GRI C2H3+H=C2H2+H2 in 1997 WangFrenklach A1CHCH=C6H4C2H3 6.40E+61 -14.59 88200.0 !1999 Davis et al. pC3H4=aC3H4 plog / 0.100 6.40E+61 -14.59 88200.0/ plog / 0.400 5.81E+62 -14.63 91211.0/ plog / 1.000 5.15E+60 -13.93 91117.0/ plog / 2.000 7.64E+59 -13.59 91817.0/

plog / 5.000 3.12E+58 -13.07 92680.0/ plog / 10.000 1.90E+57 -12.62 93300.0/ plog /100.000 1.40E+52 -10.86 95400.0/ A1CHCH+H=C6H4C2H3+H 2.30E+37 -6.00 35164.0 !1997 WangFrenklach A1CHCH+H=A1CCH2+H C6H4C2H3=o-C6H4+C2H3 6.11E+45 -8.857 94350.6 !1997 Madden et al. RRKM A1-=o-C6H4+H plog / 0.500 6.11E+45 -8.857 94350.6/ plog / 1.000 8.00E+41 -7.72 92300.3/ plog / 10.000 1.66E+30 -4.318 85756.9/

C6H4C2H3+H(+M)=A1C2H3(+M) 1.00E+14 0.0 0.0 !1997 WangFrenklach A1-+H(+M)=A1(+M) LOW / 6.60E+75 -16.30 7000.0/ TROE/ 1.0 0.1 584.9 6113.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ A1+C2H3=A1C2H3+H 7.90E+11 0.0 6400.0 !1989 FahrStein A1-+C2H4=A1C2H3+H 2.51E+12 0.0 6190.0 !1989 FahrStein in 1997 WangFrenklach A1-+C2H3=A1C2H3 1.90E+48 -10.52 17489.0 !1997 WangFrenklach RRKM plog / 0.0263 1.90E+48 -10.52 17489.0/ plog / 0.1184 3.90E+38 -7.63 12900.0/ plog / 1.0000 1.20E+27 -4.22 7200.0/ C4H4+C4H4=A1C2H3 1.50E+14 0.0 38000.0 !1984 LundgardHeicklen A1C2H3=A1CCH2+H 1.20E+46 -9.07 118323.0 !1997 WangFrenklach RRKM plog / 0.0263 1.20E+46 -9.07 118323.0/ plog / 0.1184 3.80E+37 -6.55 114200.0/ plog / 1.0000 5.30E+27 -3.63 109300.0/ A1C2H3+H=A1CCH2+H2 3.33E+05 2.53 9240.0 !HACA A1C2H3=A1CHCH+H 1.90E+54 -11.39 130224.0 !1997 WangFrenklach RRKM plog / 0.0263 1.90E+54 -11.39 130224.0/ plog / 0.1184 1.30E+44 -8.36 125400.0/ plog / 1.0000 1.10E+32 -4.77 119500.0/ A1C2H3+H=A1CHCH+H2 6.65E+05 2.53 12240.0 !GRI C2H4+H=C2H3+H2 in 1997 WangFrenklach

A1C2H3+H(+M)=A1CHCH3(+M) 1.367E+09 1.463 1355.0 !2004 MillerKlippenstein C2H4+H(+M)=C2H5(+ LOW / 2.027E+39 -6.642 5769.0/ TROE/-0.569 299.0 9147.0 -152.4/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ A1C2H3+H(+M)=A1CH2CH2(+M) 1.367E+09 1.463 1355.0 !2004 MillerKlippenstein C2H4+H(+M)=C2H5(+M) LOW / 2.027E+39 -6.642 5769.0/ TROE/-0.569 299.0 9147.0 -152.4/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ A1CH2CH2=C2H4+A1- 7.1E+14 0.0 43500.0 !bounaceur et al Int J Chem Kinet 37: 25-49, 2005 actually taken from Ebert 1978 A1CHCH3=A1CH2CH2 6.40E+61 -14.59 88200.0 !1999 Davis et al. pC3H4=aC3H4 plog / 0.100 6.40E+61 -14.59 88200.0/ plog / 0.400 5.81E+62 -14.63 91211.0/ plog / 1.000 5.15E+60 -13.93 91117.0/ plog / 2.000 7.64E+59 -13.59 91817.0/ plog / 5.000 3.12E+58 -13.07 92680.0/ plog / 10.000 1.90E+57 -12.62 93300.0/ plog /100.000 1.40E+52 -10.86 95400.0/ A1-+C4H6=A1C2H3+C2H3 3.20E+11 0.0 1900.0 !1988 Harris et al.

A1C2H5(+m) = A1CHCH3+H(+m) 2.78e+15 0.17 9.1168e+04 ! LOW/ 1.00E+98 -22.855 9.9882E+04/ TROE/6.547194E-02 1.511253E+01 9.999996E+09 7.596123E+07/ A1C2H5(+m) = A1-+C2H5(+m) 1.95E+27 -3.16 1.07447E+05 LOW/ 1.00E+98 -22.966 1.2208E+05/ TROE/7.054562E-01 9.999989E+09 4.599180E+02 8.213938E+09/ A1CH2CH2+H(+M)=A1C2H5(+M) 5.21E+17 -0.990 1580.0 !GRI3.0 C2H5+H(+M)=C2H6(+M) LOW / 1.99E+41 -7.080 6685.0/ TROE/ 0.8422

125.0 2219.00 6882.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ A1CH2+CH3(+M)=A1C2H5(+M) 6.120E+16 -0.970 620.00 != CH3+CH3(+M)=C2H6(+M) LOW / 1.770E+50 -9.670 6220.0/ ! TROE/ 0.5325 151.0 1038.00 4970.0/ H2/2.0/ CH4/2.0/ C2H6/3.0/ AR/0.7/ A1CH2+CH3=A1CHCH3+H 1.730e+039 -7.2310 35366.0 ! Miyoshi 2012 rev / 2.210e+039 -6.8522 24335.7 / A1CH2+CH3=A1CH2CH2+H 6.348e+032 -5.1046 40697.1 ! Miyoshi 2012 rev / 1.169e+031 -4.6094 14826.4 / A1CH2+CH3=A1- +C2H5 2.028e+033 -5.2232 40498.3 ! Miyoshi 2012 rev / 3.313e+032 -5.4269 14897.5 / A1CHCH3+H=A1CH2CH2 1.614e+024 -2.5623 29906.1 ! Miyoshi 2012 rev / 2.325e+022 -2.4459 15065.6 / A1CHCH3+H=A1- +C2H5 5.150e+024 -2.6808 29738.4 ! Miyoshi 2012 rev / 6.584e+023 -3.2634 15168.0 / A1CH2CH2+H=A1- +C2H5 6.974e+014 0.0003 17190.1 ! Miyoshi 2012 rev / 6.181e+015 -0.6985 17459.8 / A1C2H5+H=A1CHCH3+H 3.31E+07 2.0 5345.3 !2005 Baulch et al. A1C2H5+H=A1CH2CH2+H2 7.22E+08 1.50 7412.0 !2005 Baulch et al. A1C2H5+CH3=A1CHCH3+CH4 1.1E+12 0.0 9100.0 !Bounaceur et al 2005 Int J Chem Kinet 37: 25-49 A1C2H5+CH3=A1CH2CH2+CH4 0.3 4.0 8200.0 !Bounaceur et al 2005 Int J Chem Kinet 37: 25-49 A1C2H5+H=A1+C2H5 1.20E+13 0.0 5100.0 !Ergut et al 2006 Combustion and Flame 144 (2006) 757-772 A1C2H5+H=C6H4C2H5+H2 1.93E+07 2.00 9697.0 !2005 Baulch et al.

!**********IPCH sub mechanism****

! isomerization and decomposition of IPCH IPCH = cC6H11+iC3H7 1.47E+16 0.0 81449.4 !barrierless IPCH = SXC2H4cC6H11+CH3 4.23E+15 0.0 80690.3 !barrierless!2nd-HR3 IPCH = int1 1.11E+16 0.0 88829.8 IPCH = int2 2.75E+15 0.0 91017.7 IPCH = int3 4.33E+16 0.0 90940.2

int1 = C8H15-1E7M 4.23E+10 0.0 4084.1 int1 = C8H15-3E2M 1.05E+12 0.0 2965.3 int1 = C8H15-2E2M 1.84E+10 0.0 15967.7

int2 = C6H11-1E2IP 3.21E+11 0.0 7516.6 int2 = C6H11-1E5IP 3.51E+11 0.0 6783.7

int3 = C6H11-1E3IP 4.02E+10 0.0 13908.2 int3 = C6H11-1E4IP 9.76E+11 0.0 4949.7

! CH3-abstractions of IPCH IPCH+H = SXC2H4cC6H11+CH4 1.71E+14 0.0 35590.8

! H-abstractions of IPCH IPCH+H = PXIPCH+H2 5.86E+14 0.0 13805.7 IPCH+H = TX- IPCH+H2 1.61E+14 0.0 8684.7 IPCH+H = T1XIPCH+H2 1.15E+14 0.0 8663.2 IPCH+H = S2XIPCH+H2 4.21E+14 0.0 11389.8 IPCH+H = S3XIPCH+H2 6.40E+14 0.0 11125.9 IPCH+H = S4XIPCH+H2 3.42E+14 0.0 11391.8

IPCH+CH3 = PXIPCH+CH4 7.37E+12 0.0 19247.8 IPCH+CH3 = TXIPCH+CH4 4.23E+12 0.0 14469.2 IPCH+CH3 = T1XIPCH+CH4 2.40E+12 0.0 14369.8 IPCH+CH3 = S2XIPCH+CH4 3.57E+12 0.0 17063.3 IPCH+CH3 = S3XIPCH+CH4 1.45E+13 0.0 16647.6 IPCH+CH3 = S4XIPCH+CH4 8.26E+12 0.0 16918.2

!cyclohexyl radicals PXIPCH = CH2-IPCH+H 6.00E+13 0.0 36558.5 TXIPCH = CH2-IPCH+H 1.09E+14 0.0 38837.8 !barrierless TXIPCH = CH2-2-IPCH+H 6.73E+14 0.0 40203.0 T1XIPCH = CH2-2-IPCH+H 5.33E+13 0.0 36975.8 T1XIPCH = IPCH-1E+H 3.04E+14 0.0 37065.3 S2XIPCH = IPCH-1E+H 3.72E+13 0.0 35986.2 S2XIPCH = IPCH-2E+H 2.73E+14 0.0 36898.3 S3XIPCH = IPCH-2E+H 1.88E+14 0.0 37748.9 S3XIPCH = IPCH-3E+H 2.20E+14 0.0 37587.9 S4XIPCH = IPCH-3E+H 2.53E+14 0.0 36087.6 SXC2H4cC6H11 = CH2CHcC6H11+H 2.75E+13 0.0 38245.7 !barrierless SXC2H4cC6H11 = CH3CHcC6H10+H 2.17E+13 0.0 37820.4 PXIPCH = CH2CHcC6H11+CH3 2.67E+14 0.0 31415.6 PXIPCH = cC6H11+C3H6 1.68E+14 0.0 26950.4 T1XIPCH = CH3CHcC6H10+CH3 1.64E+14 0.0 30616.8 S2XIPCH = cC6H10+iC3H7 0.92E+14 0.0 27693.6

TXIPCH = P8XC8H14-2E2M 2.97E+14 0.0 30897.0 T1XIPCH = P6XC6H10-1E2IP 0.75E+14 0.0 31662.1 S2XIPCH = P6XC6H10-1E3IP 0.64E+14 0.0 31111.6 S2XIPCH = P8XC8H14-3E2M 0.69E+14 0.0 30306.8 S3XIPCH = P6XC6H10-1E4IP 1.22E+14 0.0 32524.5 S3XIPCH = S6XC8H14-1E7M 0.73E+14 0.0 29120.4 S4XIPCH = P6XC6H10-1E5IP 1.98E+14 0.0 32204.6

!cyclohexene dissociation IPCH-1E = C2H4+C4H5-13E2IP 1.87E+15 0.0 65045.0 IPCH-2E = C2H4+C6H9-13E5M 1.15E+15 0.0 62642.5 IPCH-3E = C4H6+C4H7-1E3M 8.08E+14 0.0 64774.8

alkenes reactions

C8H15-1E7M+H = S3XC8H14-1E7M+H2 2.24E+14 0.0 8247.1 C8H15-1E7M+CH3 = S3XC8H14-1E7M+CH4 4.65E+08 0.0 8374.6 C8H15-1E7M = C3H6+C5H9-1E4M 4.95E+12 0.0 55419.0 C8H15-1E7M = aC3H5+P1XC5H104M 1.33E+14 0.0 63602.3 !barrierless

C8H15-3E2M+H = S5XC8H14-3E2M+H2 2.42E+11 0.0 5397.4 C8H15-3E2M+CH3 = S5XC8H14-3E2M+CH4 3.18E+12 0.0 13386.4 C8H15-3E2M = C3H6+C5H9-2E4M 1.16E+15 0.0 109252.3 C8H15-3E2M = C3H6+C5H9-1E4M 5.73E+12 0.0 56961.1 C8H15-3E2M = nC3H7+P1XC5H8-2E4M 1.90E+15 0.0 68572.3 !barrierless

C8H15-2E2M+H = S4XC8H14-2E2M+H2 2.40E+14 0.0 7480.4 C8H15-2E2M+CH3 = S4XC8H14-2E2M+CH4 1.91E+12 0.0 12610.4 C8H15-2E2M = C4H8-1+C4H7-2E2M 1.95E+15 0.0 108489.2 C8H15-2E2M = C4H8-1+C4H7-1E3M 5.31E+12 0.0 57507.6 C8H15-2E2M = pC4H9+P4XC4H6-2E2M 2.25E+15 0.0 66191.6 !barrierless

C6H11-1E2IP+H = S3XC6H10-1E2IP+H2 1.56E+14 0.0 7994.9 C6H11-1E2IP+CH3 = S3XC6H10-1E2IP+CH4 1.14E+12 0.0 13017.4 C6H11-1E2IP = C3H6+C4H6-1E23M 6.59E+12 0.0 55162.7 C6H11-1E2IP = nC3H7+P1XCH2C4H6-1E3M 2.09E+15 0.0 66986.5 !barrierless

C6H11-1E5IP+H = S3XC6H10-1E5IP+H2 5.10E+15 0.0 11236.2 C6H11-1E5IP+CH3 = S3XC6H10-1E5IP+CH4 4.10E+13 0.0 16489.6 C6H11-1E5IP = C3H6+C4H6-1E23M 1.11E+14 0.0 55272.0

C6H11-1E5IP = aC3H5+P1XC4H723M 3.72E+16 0.0 69110.8 !barrierless

C6H11-1E3IP+H = T3XC6H10-1E3IP+H2 2.22E+14 0.0 8814.2 C6H11-1E3IP+CH3 = T3XC6H10-1E3IP+CH4 1.24E+12 0.0 14405.2 C6H11-1E3IP = C3H6+C5H9-2E4M 3.97E+12 0.0 53586.8 C6H11-1E3IP = C3H6+C6H12-2E 2.91E+13 0.0 55132.9 C6H11-1E3IP = iC3H7+S3XC6H11-1E 6.19E+14 0.0 62634.6 !barrierless C6H11-1E3IP = nC3H7+S3XC5H8-1E4M 1.65E+14 0.0 64625.7 !barrierless

C6H11-1E4IP+H = S3XC6H10-1E4IP+H2 2.13E+14 0.0 9020.5 C6H11-1E4IP+CH3 = S3XC6H10-1E4IP+CH4 1.24E+12 0.0 14520.7 C6H11-1E4IP = C3H6+C5H9-2E2M 2.55E+15 0.0 104278.3 C6H11-1E4IP = C3H6+C5H9-2E4M 7.33E+12 0.0 57563.2 C6H11-1E4IP = aC3H5+S3XC5H102M 3.20E+14 0.0 63175.1 !barrierless

Alkyl RAdical reactions

S6XC8H14-1E7M = S7XC8H14-1E7M 8.86E+12 0.0 39591.0 S6XC8H14-1E7M = S5XC8H14-1E7M 5.99E+12 0.0 40073.9 S6XC8H14-1E7M = S4XC8H14-1E7M 3.75E+12 0.0 41288.1 S6XC8H14-1E7M = S3XC8H14-1E7M 1.70E+11 0.0 19827.5 S6XC8H14-1E7M = P8XC8H14-1E7M 5.24E+12 0.0 43070.8

S7XC8H14-1E7M = iC4H8+P5XC5H9-1E 1.61E+15 0.0 64774.8 S6XC8H14-1E7M = CH3+C8H14-16E 5.02E+13 0.0 31473.3 S6XC8H14-1E7M = C4H7-1E3M+C4H7 1.76E+14 0.0 31270.8 S5XC8H14-1E7M = iC3H7+C6H10-15E 1.13E+14 0.0 29438.4 S5XC8H14-1E7M = aC3H5+C5H9-1E4M 2.64E+13 0.0 22944.2 S4XC8H14-1E7M = iC4H9+C5H8-14E 1.43E+14 0.0 31604.4 S4XC8H14-1E7M = C2H3+C6H11-1E5M 1.89E+14 0.0 38619.2 S3XC8H14-1E7M = C4H6+P4XC4H83M 1.12E+15 0.0 39587.0 P8XC8H14-1E7M = CH3+C8H14-17E 2.51E+14 0.0 33953.3 P8XC8H14-1E7M = C3H6+P6XC6H11-1E 2.57E+14 0.0 31562.7

S6XC8H14-1E7M = P1XCH2cC5H85IP 2.09E+10 0.0 7160.5

P8XC8H14-2E2M = S7XC8H14-2E2M 4.25E+13 0.0 40614.4 P8XC8H14-2E2M = S6XC8H14-2E2M 1.62E+13 0.0 40064.0 P8XC8H14-2E2M = S5XC8H14-2E2M 1.97E+12 0.0 23242.3 P8XC8H14-2E2M = S4XC8H14-2E2M 1.50E+11 0.0 13043.8 S7XC8H14-2E2M = C3H6+P5XC5H8-2E2M 1.33E+14 0.0 29919.3 S6XC8H14-2E2M = CH3+C7H11-15E6M 5.43E+13 0.0 31650.1 S6XC8H14-2E2M = C4H8-1+P4XC4H6-2E2M 1.80E+13 0.0 21177.6 S5XC8H14-2E2M = iC4H7-1+C5H10-1E 1.18E+14 0.0 38341.0 S5XC8H14-2E2M = C2H5+C6H9-14E5M 9.41E+13 0.0 30410.1 S4XC8H14-2E2M = nC3H7+C5H7-13E4M 1.31E+15 0.0 40040.1 P8XC8H14-2E2M = C2H4+P6XC6H10-2E2M 3.42E+14 0.0 30662.5

P8XC8H14-3E2M = S7XC8H14-3E2M 2.30E+13 0.0 40525.0 P8XC8H14-3E2M = S6XC8H14-3E2M 1.02E+13 0.0 40827.0 P8XC8H14-3E2M = S5XC8H14-3E2M 8.23E+11 0.0 18331.7

S7XC8H14-3E2M = C3H6+P1XC5H8-2E4M 3.36E+13 0.0 21660.5 S6XC8H14-3E2M = C7H11-14E6M+CH3 8.11E+13 0.0 31922.4 S6XC8H14-3E2M = C4H8-1+S1XC4H6-1E3M 2.46E+14 0.0 39070.3

S5XC8H14-3E2M = C2H5+C6H9-13E5M 4.59E+14 0.0 40185.2 !P8XC8H14-3E2M = C2H4+P1XC6H10-3E5M 2.93E+14 0.0 31433.5 P8XC8H14-3E2M = S1XIPcC5H9 2.24E+11 0.0 8455.7

P6XC6H10-1E5IP = T5XC6H10-1E5IP 4.09E+13 0.0 38585.5 P6XC6H10-1E5IP = S4XC6H10-1E5IP 2.56E+13 0.0 39920.7 P6XC6H10-1E5IP = S3XC6H10-1E5IP 1.27E+12 0.0 17639.2

T5XC6H10-1E5IP = C7H11-15E5M+CH3 1.18E+14 0.0 31177.2 T5XC6H10-1E5IP = C4H6-1E23M+aC3H5 6.05E+13 0.0 21280.9 S4XC6H10-1E5IP = C7H11-14E6M+CH3 4.90E+13 0.0 32027.7 S4XC6H10-1E5IP = C6H10-14E+iC3H7 2.87E+13 0.0 25664.7 S4XC6H10-1E5IP = C5H8-1E34M+C2H3 3.18E+14 0.0 38345.0 S3XC6H10-1E5IP = S2XC4H83M+C4H6 7.87E+14 0.0 38092.6 P6XC6H10-1E5IP = iC3H7+C6H10-15E 1.16E+14 0.0 25903.2 P6XC6H10-1E5IP = C4H7-1E3M+C4H7 1.56E+14 0.0 29519.9

P6XC6H10-1E5IP = P1XCH2cC5H84IP 2.03E+11 0.0 6033.9

P6XC6H10-1E4IP = T4XC6H10-1E4IP 6.24E+14 0.0 39197.5 P6XC6H10-1E4IP = S5XC6H10-1E4IP 2.09E+15 0.0 42259.8 P6XC6H10-1E4IP = S3XC6H10-1E4IP 2.23E+13 0.0 22254.7

!T4XC6H10-1E4IP = C6H9-14E4Et+CH3 9.21E+13 0.0 31026.2 T4XC6H10-1E4IP = C5H7-14E2IP+CH3 1.30E+14 0.0 31268.6 T4XC6H10-1E4IP = C4H7-1E2IP+C2H3 6.44E+14 0.0 39273.0 S5XC6H10-1E4IP = C6H10-14E+iC3H7 6.17E+13 0.0 26807.3 S5XC6H10-1E4IP = C5H9-2E4M+aC3H5 1.16E+13 0.0 19403.6 S3XC6H10-1E4IP = C6H10-13E+iC3H7 1.82E+14 0.0 33470.4 S3XC6H10-1E4IP = C6H9-13E5M+C2H5 1.36E+14 0.0 37530.3 P6XC6H10-1E4IP = S4XC6H10-1E5M+C2H4 1.18E+14 0.0 31177.2

P6XC6H10-1E4IP = P1XCH2cC5H84IP 1.23E+13 0.0 8551.9

P6XC6H10-1E3IP = T3XC6H10-1E3IP 2.39E+11 0.0 18305.3 P6XC6H10-1E3IP = S5XC6H10-1E3IP 2.81E+13 0.0 40542.9 P6XC6H10-1E3IP = S4XC6H10-1E3IP 4.53E+12 0.0 38309.2

T3XC6H10-1E3IP = C5H7-13E3C3H7+CH3 4.74E+14 0.0 39004.8 T3XC6H10-1E3IP = C4H5-13E2IP+C2H5 3.04E+15 0.0 40562.7 S5XC6H10-1E3IP = S3XC5H8-1E4M+C3H6 4.51E+13 0.0 21133.9 S4XC6H10-1E3IP = C6H11-3E2M+C2H3 1.91E+14 0.0 38627.2 S4XC6H10-1E3IP = C6H10-

13E+iC3H7 2.20E+13 0.0 24969.2 S4XC6H10-1E3IP = C5H7-14E3IP+CH3 5.02E+13 0.0 31679.9 P6XC6H10-1E3IP = P4XC4H6-1E3IP+C2H4 1.40E+14 0.0 30376.3

P6XC6H10-1E3IP = P1XCH2cC5H85IP 2.51E+10 0.0 9310.4

P6XC6H10-1E2IP = S5XC6H10-1E2IP 2.41E+13 0.0 40515.0 P6XC6H10-1E2IP = S4XC6H10-1E2IP 9.13E+12 0.0 39644.6 P6XC6H10-1E2IP = S3XC6H10-1E2IP 5.31E+11 0.0 18726.6

S5XC6H10-1E2IP = C3H6+P3XC3H4-1E2IP 4.47E+13 0.0 21378.3 S4XC6H10-1E2IP = C5H7-14E2IP+CH3 7.69E+13 0.0 31805.1 S4XC6H10-1E2IP = C4H8-1+T2XC4H6-1E3M 1.17E+14 0.0 35322.5 S3XC6H10-1E2IP = C4H5-13E2IP+C2H5 5.45E+13 0.0 36155.1 P6XC6H10-1E2IP = C2H4+P4XC4H6-1E2IP 2.70E+14 0.0 30483.6

P6XC6H10-1E2IP = P1XCH2cC5H81IP 3.08E+10 0.0 7584.9

cyclopentane reactions

S1XIPcC5H9 = T3XcC5H8CH2IP 5.37E+10 0.0 29160.2 T3XcC5H8CH2IP = cC5H7-3ECH2IP+H 8.33E+13 0.0 38714.6 cC5H7-3ECH2IP+H = S2XcC5H6-3ECH2IP+H2 2.42E+14 0.0 8338.9 cC5H7-3ECH2IP+CH3 = S2XcC5H6-3ECH2IP+CH4 4.20E+12 0.0 13266.1 S2XcC5H6-3ECH2IP = C5H6+iC4H9 7.26E+14 0.0 38611.3

P1XCH2cC5H85IP = S3XcC5H71M5IP 1.12E+12 0.0 25833.6 P1XCH2cC5H85IP = S4XcC5H71M5IP 1.78E+12 0.0 25978.7

S3XcC5H71M5IP = cC5H61M5IP+H 7.27E+13 0.0 38058.9 cC5H61M5IP+H = S1XcC5H65IP+CH4 2.54E+14 0.0 33613.5 S1XcC5H65IP = C5H6+iC3H7 3.23E+14 0.0 34784.0 S4XcC5H71M5IP = cC5H75M+iC3H7 1.31E+14 0.0 26121.7

cC5H75M+H = cC5H71-3+CH4 6.64E+13 0.0 32210.5

!cC5H75M+H = cC5H7+CH4 6.64E+13 0.0 32210.5 cC5H75M+H = S3XcC5H65M+H2 1.36E+14 0.0 5527.6 cC5H75M+CH3 = S3XcC5H65M+CH4 2.16E+12 0.0 11079.8 S3XcC5H65M = cC5H5-13E5M+H 1.31E+14 0.0 49034.2 !barrierless

P1XCH2cC5H84IP = S3XcC5H71M4IP 1.16E+12 0.0 26229.1 S3XcC5H71M4IP = cC5H74M+iC3H7 1.30E+14 0.0 25487.8 cC5H74M+H = S3XcC5H64M+H2 1.24E+14 0.0 7292.9 cC5H74M+CH3 = S3XcC5H64M+CH4 2.30E+12 0.0 12824.8 S3XcC5H64M = C5H6+CH3 4.34E+14 0.0 39489.6 S3XcC5H64M = cC5H5-13E1M+H 9.76E+13 0.0 45890.4

P1XCH2cC5H81IP = S3XcC5H71M1IP 1.00E+12 0.0 24812.2 S3XcC5H71M1IP = cC5H61M1IP+H 1.02E+14 0.0 38311.2 cC5H61M1IP+H = S2XcC5H51M1IP+H2 4.03E+14 0.0 7510.4 cC5H61M1IP+CH3

= S2XcC5H51M1IP+CH4 3.36E+12 0.0 12659.1 S2XcC5H51M1IP = cC5H5-13E1M+iC3H7 1.46E+14 0.0 32685.5

cC5H5-13E5M = cC5H5-13E1M 1.50E+13 0.0 24466.4

aromatic reactions

IPCH-1E+H = S6XIPCH-1E+H2 2.69E+14 0.0 7009.3 S6XIPCH-1E = IPCH-15E+H 5.79E+14 0.0 50564.3 IPCH-15E+H = S4XIPCH-15E+H2 3.52E+14 0.0 6674.4 IPCH-15E+H = S3XIPCH-15E+H2 3.61E+14 0.0 6350.3 S4XIPCH-15E = A1IP+H 1.72E+14 0.0 30390.3 S3XIPCH-15E = A1IP+H 1.24E+14 0.0 30322.7 A1IP+H = PXA1IP+H2 9.31E+14 0.0 13611.3 PXA1IP = A1-+C3H6 1.14E+15 0.0 40940.3 PXA1IP = A1C2H3+CH3 6.33E+14 0.0 32466.9 IPCH-2E+H = T1XIPCH-2E+H2 1.33E+14 0.0 5993.2 T1XIPCH-2E = IPCH-15E+H 1.81E+14 0.0 48074.3 IPCH-3E+H = S2XIPCH-3E+H2 1.20E+14 0.0 7417.4 S2XIPCH-3E = IPCH-13E+H 1.35E+14 0.0 49221.0 S2XIPCH-3E = cC6H8-13E+iC3H7 5.49E+14 0.0 39370.4 IPCH-13E+H = S5XIPCH-13E+H2 4.85E+14 0.0 10420.5 IPCH-13E+H = S6XIPCH-13E+H2 2.88E+14 0.0 6558.0 S5XIPCH-13E = A1IP+H 1.94E+14 0.0 30296.9 S6XIPCH-13E = A1IP+H 1.74E+14 0.0 30225.3

additional reactions

C4H7-1E3M+H = SAXC4H7+CH4 1.71E+14 0.0 35590.8 !IPCH+H = SXC2H4cC6H11+CH4 rxn

P4XC4H6-2E2M+H = C4H7-2E2M 1.33E+13 0.0 3260.7 ! =(C3H6+H=nC3H7) TS5 600 cm-1 USC Mech V2.0 !iC4H8+H(+M) = iC4H9(+M)

C4H7-2E2M+H = CH3CCHCH3+CH4 1.71E+14 0.0 35590.8 !IPCH+H = SXC2H4cC6H11+CH4 rxn

P4XC4H83M = C3H6+C2H5 2.57E+14 0.0 31562.7 ! P8XC8H14-1E7M = C3H6+P6XC6H11-1E

S2XC4H83M = CH3+C4H8-2 5.02E+13 0.0 31473.3 !S6XC8H14-1E7M = CH3+C8H14-16E

S3XC5H102M = C5H10-2E+CH3 5.02E+13 0.0 31473.3 !S6XC8H14-1E7M = CH3+C8H14-16E S3XC5H102M = C4H7-1E3M+CH3 5.02E+13 0.0 31473.3 !S6XC8H14-1E7M = CH3+C8H14-16E

S3XC5H8-1E4M = CH3+C5H8-13E 5.02E+13 0.0 31473.3 !S6XC8H14-1E7M = CH3+C8H14-16E

P5XC5H8-2E2M = C2H4+CH3CCHCH3 1.89E+14 0.0 38619.2 !S4XC8H14-1E7M = C2H3+C6H11-1E5M

P1XCH2C4H6-1E3M = aC3H4+iC3H7 2.20E+13 0.0 24969.2 !S4XC6H10-1E3IP = C6H10-13E+iC3H7

P1XC5H8-2E4M+H = C5H9-2E4M 1.33E+13 0.00 3260.7 ! =(C3H6+H=nC3H7) TS5 600 cm-1 USC Mech V2.0 !iC4H8+H(+M) = iC4H9(+M)

C5H7-13E4M+H = T4XC5H7-13E+CH4 1.71E+14 0.0 35590.8 !IPCH+H = SXC2H4cC6H11+CH4 rxn

C5H9-1E4M+H = S4XC5H9-1E+CH4 1.71E+14 0.0 35590.8 !IPCH+H = SXC2H4cC6H11+CH4 rxn

C5H9-2E4M+H = S4XC5H9-2E+CH4 1.71E+14 0.0 35590.8 !IPCH+H = SXC2H4cC6H11+CH4 rxn

C4H6-1E23M = CH3CCH2+iC3H7 1.33E+14 0.0 63602.3 !C8H15-1E7M = aC3H5+P1XC5H104M

C4H6-1E23M = C3H6+C3H6 8.0E+05 1.81 53454 ! ! C5H9-1E4M = C3H6+C3H6 PLOG / 0.039 8.0E+05 1.81 53454/ ! 1.62E+06 /20 EST PLOG / 1 1.62E+06 1.81 53454/ ! 08/TSAwip JetSurF 2.0

C4H5-13E2IP = iC4H5+iC3H7 1.33E+14 0.0 63602.3 !C8H15-1E7M = aC3H5+P1XC5H104M

C4H7-1E2IP = C4H7-2+iC3H7 1.33E+14 0.0 63602.3 !C8H15-1E7M = aC3H5+P1XC5H104M

C6H9-14E5M = aC3H5+iC4H7-1 1.33E+14 0.0 63602.3 !C8H15-1E7M = aC3H5+P1XC5H104M

P4XC4H6-1E2IP = C2H4+T2XC4H6-1E3M 1.89E+14 0.0 38619.2 !S4XC8H14-1E7M = C2H3+C6H11-1E5M T2XC4H6-1E3M+H = C4H7-1E3M 1.33E+13 0.0 3260.7 ! =(C3H6+H=nC3H7) TS5 600 cm-1 USC Mech V2.0 !iC4H8+H(+M) = iC4H9(+M)

P4XC4H6-1E3IP = C4H6+iC3H7 2.20E+13 0.0 24969.2 !S4XC6H10-1E3IP = C6H10-13E+iC3H7

P6XC6H10-2E2M = C2H4+P4XC4H6-2E2M 3.42E+14 0.0 30662.5 ! P8XC8H14-2E2M = C2H4+P6XC6H10-2E2M

S4XC6H10-1E5M = C2H3+C4H7-1E3M 1.89E+14 0.0 38619.2 !S4XC8H14-1E7M = C2H3+C6H11-1E5M

C5H7-14E2IP = aC3H5+T2XC4H6-1E3M 1.33E+14 0.0 63602.3 !C8H15-1E7M = aC3H5+P1XC5H104M

C5H7-13E3C3H7 = C3H6+C5H8-13E 4.95E+12 0.0 55419.0 !C8H15-1E7M = C3H6+C5H9-1E4M

P4XC4H6-2E2M = C4H5-13E2M+H 1.27E+24 -4.75 23777 ! Ref to C4H7 = C4H6+H PLOG / 0.033 1.27E+24 -4.75 23777/ PLOG / 0.066 1.38E+26 -5.221 25729/ PLOG / 0.132 1.75E+28 -5.709 27764/ PLOG / 0.197 3.16E+29 -6.003 28985/ PLOG / 0.263 2.69E+30 -6.222 29890/ PLOG / 1.0 2.48E+53 -12.30 52000/ PLOG / 10 1.85E+48 -10.50 51770/

C8H14-16E = C3H6+C5H8-13E 3.97E+12 0.0 53586.8 !C6H11-1E3IP = C3H6+C5H9-2E4M

C4H7-1E3M = C2H4+C3H6 3.97E+12 0.0 53586.8 !C6H11-1E3IP = C3H6+C5H9-2E4M

!**********Cylopentane mechanism*******!

!***UNIMOLECULAR DECOMPOSITION***

cC5H10¡=¿C5H10-1E 1.26E16 0.00 84850 cC5H10¡=¿C2H4+C3H6 1.78E16 0.00 95070 cC5H9+H¡=¿cC5H10 1E+14 0.00 0.00

!***H-ABSTRACTION*** cC5H10+H¡=¿cC5H9+H2 6.50E+06 2.40 4471 cC5H10+CH3¡=¿cC5H9+CH4 7.55 3.46 5481 cC5H10+C2H5¡=¿cC5H9+C2H6 2.50E+11 0.00 10400

!***BETA-SCISSION*** cC5H9¡=¿cC5H8+H 8.84E+11 0.694 36624.5 ! ab initio computations CCSDT/PVTZ (MJR) PLOG/ 0.01 1.40E+66 -17 51500 / ! PLOGs calculated using Wang's falloff PLOG/ 0.1 2.40E+57 -14 49500 / ! DEG=4 PLOG/ 1 2.00E+55 -13 41000 / PLOG/ 5 2.40E+49 -11 50000 / PLOG/ 10 4.44E+49 -11 50800 / PLOG/ 20 1.320E+43 -9 48000 / cC5H9¡=¿P5XC5H9-1E 1.24E+13 0.244 36044.4 ! ab initio computations CCSDT/PVTZ (MJR) PLOG/ 0.01 2.80E+74 -19.8 52500 / ! PLOGs calculated using Wang's falloff PLOG/ 0.1 2.20E+73 -19 55000 / ! DEG=2 PLOG/ 1 8.00E+62 -15.5 52500 / PLOG/ 5 2.40E+50 -11.5 48500 / PLOG/ 10 6.00E+45 -10 47300 / PLOG/ 20 2.40E+44 -9.5 47300 /

!***CYCLOPENTENE REACTIONS*** !cC5H8¡=¿C5H8D14 5.04E15 0.00 96850 cC5H8¡=¿C5H8-13E 5.06E15 0.00 6.6E+04 cC5H8¡=¿C2H2+C3H6 7.12E15 0.00 107067 cC5H8¡=¿C5H6+H2 2.24E13 0.0 60000

cC5H8+H¡=¿cC5H71-4+H2 1.3E+06 2.4 4.471E+03 cC5H8+CH3¡=¿cC5H71-4+CH4 1.51 3.5 5.481E+03 cC5H8+C2H5¡=¿cC5H71-4+C2H6 5E+10 0.0 10400 cC5H8+H¡=¿cC5H71-3+H2 6.752E+05 2.36 2.070E+02 cC5H8+CH3¡=¿cC5H71-3+CH4 7.380E+00 3.31 4.002E+03 cC5H8+C2H5¡=¿cC5H71-3+C2H6 2.97 3.5 6637 cC5H8+H¡=¿cC5H71-2+H2 6.752E+05 2.36 2.070E+02 cC5H8+CH3¡=¿cC5H71-2+CH4 7.380E+00 3.31 4.002E+03 cC5H8+C2H5¡=¿cC5H71-2+C2H6 2.97 3.5 6637

! BETA SCISSION OF CYCLOPENTYL RADICALS cC5H71-3¡=¿P5XC5H7-13E 9.6E8 1.05 5570 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA DECREASED BY 13.2 KCAL, ENERGY DIFF. BETWEEN VINYL-SEC AND SEC-SEC C-C BONDS cC5H71-4¡=¿T1XC5H7-14E 9.6E8 1.05

5570 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA DECREASED BY 13.2 KCAL, ENERGY DIFF. BETWEEN VINYL-SEC AND SEC-SEC C-C BONDS P5XC5H7-13E+H¡=¿C5H8-13E 8.48E+11 0.51 1230 T1XC5H7-14E+H¡=¿C5H8-14E 8.48E+11 0.51 1230

!C5H714-1¡=¿CYC5H71-4 9.6E8 1.05 5570 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA DECREASED BY 13.2 KCAL, ENERGY DIFF. BETWEEN VINYL-SEC AND SEC-SEC C-C BONDS !C5H6+H¡=¿CYC5H71-4 8.41E11 0.51 1230 ! ANALOGY WITH H+C3H6=IC3H7 CURRAN 2006 (DEG=2) !CVCCVCCJ¡=¿CYC5H71-3 6.14E10 1.05 23850 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA INCREASED BY 8.05 KCAL, THE STABILIZATION ENERGY OF DOUBLE RESONANCE COMPARED TO SINGLE RES. !C5H6+H¡=¿CYC5H71-3 8.48E+11 0.51 1230 ! ANALOGY WITH H+C3H6=IC3H7 CURRAN 2006 (DEG=2)

Decalin mechanism*****

!Unimolecular decomposition and isomerization of decalin

decalin = S2Xdecalin+H 4.65E+15 0.0 102378.6 decalin = S3Xdecalin+H 2.84E+16 0.0 102114.3 decalin = T1Xdecalin+H 3.13E+15 0.0 99757.4 decalin = biradical1 8.21E+17 0.0 90485.2 decalin = biradical2 2.92E+17 0.0 89428.0 decalin = biradical3 2.92E+17 0.0 92329.3 biradical1 = C6H10-1E56CH 2.92E+17 0.0 92329.3 biradical2 = C6H10-1E45CH 3.52E+11 0.0 4045.3 biradical3 = C6H10-1E34CH 2.76E+12 0.0 4419.7

!abstraction reaction by H atom and CH3 radical

decalin + H = S2Xdecalin + H2 1.34E+15 0.0 11023.2 decalin + H = S3Xdecalin + H2 1.48E+15 0.0 11258.3 decalin + H = T1Xdecalin + H2 2.66E+14 0.0 8556.9 decalin + CH3 = S2Xdecalin + CH4 1.80E+13 0.0 16449.0 decalin + CH3 = S3Xdecalin + CH4 3.40E+13 0.0 16798.8 decalin + CH3 = T1Xdecalin + CH4 3.78E+12 0.0 14134.4

!decomposition and isomerization of decalin radicals

T1Xdecalin = decalin-1bE+H 2.81E+14 0.0 35378.1 T1Xdecalin = decalin-1E+H 3.94E+14 0.0 37802.5 S2Xdecalin = decalin-1E+H 6.30E+13 0.0 36745.3 S2Xdecalin = decalin-2E+H 2.21E+14 0.0 38132.4 S3Xdecalin = decalin-2E+H 2.27E+14 0.0 38364.9 S3Xdecalin = decalin-3E+H 2.85E+14 0.0 37991.3 T1Xdecalin = P6XC6H9-1E23CH 3.60E+14 0.0 36165.1 T1Xdecalin = P6XC6H9-1E12CH 1.81E+14 0.0 32888.2 S3Xdecalin = S6XC6H9-1E56CH 6.68E+13 0.0 31715.7 S3Xdecalin = P6XC6H9-1E45CH 1.07E+14 0.0 32631.8 S2Xdecalin = S6XcC10H17-1E 5.16E+13 0.0 30459.8 S2Xdecalin = P4XC4H8cC6H9 1.97E+14 0.0 37252.1 S2Xdecalin = P6XC6H9-1E34CH 9.66E+13 0.0 31735.6

!decomposition and isomerization of alkenyl-cyclohexane radicals

P4XC4H8cC6H9 = TXC4H9cC6H8 3.75E+11 0.0 10156.4 P4XC4H8cC6H9 = S1XC4H8cC6H9 1.60E+12 0.0 13057.7 P4XC4H8cC6H9 = PXC2H4cC6H9-2E + C2H4 1.99E+14 0.0 29847.7 S1XC4H8cC6H9 = C2H3cC6H9-2E+C2H5 3.72E+13 0.0 35986.2 TXC4H9cC6H8 = CH2cC6H8-2E + nC3H7 8.62E+14 0.0 38609.3 TXC4H9cC6H8 = nC4H9cC6H7 + H 3.51E+03 0.0 2471.9 S1XC4H8cC6H9 = P1XC10H17-46E 1.30E+13 0.0 28456.7 S1XC4H8cC6H9 = S1XC10H17-16E 3.12E+13 0.0 53743.8 TXC4H9cC6H8 = P1XC9H15-3E5CH2 1.08E+14 0.0 44030.4 P6XC6H9-1E12CH = S1XC6H9-1E12CH 9.77E+11 0.0 18147.9 S1XC6H9-1E12CH = C2H3cC6H9 + C2H5 2.96E+14 0.0 36477.0 P6XC6H9-1E12CH = PXC2H4cC6H9-1E + C2H4 2.40E+14 0.0 16823.8 P6XC6H9-1E12CH = S1Xspiro-4-5-DN 1.36E+11 0.0 9447.5 P6XC6H9-1E23CH = T3XC6H9-1E23CH 7.27E+13 0.0 19351.8 P6XC6H9-1E23CH = PXCH2CH2cC6H9 + C2H4 8.05E+15 0.0 32770.9 T3XC6H9-1E23CH = CH2-12-cC6H8 + C2H5 2.56E+16 0.0 43446.2 T3XC6H9-1E23CH = P1XC8H13-45-CH2 5.02E+15 0.0 47617.3 P6XC6H9-1E23CH = P1XCH2-1-HD 1.27E+13 0.0 15556.6 P6XC6H9-1E34CH = T3XC6H9-1E34CH 6.56E+11 0.0 22717.7 P6XC6H9-1E34CH = CH2CH-2-cC6H10 + C2H4 1.43E+14 0.0 28603.8 T3XC6H9-1E34CH = C2H3cC6H9 + C2H5 7.96E+14 0.0 37377.2 T3XC6H9-1E34CH = P8XC8H14-3E4C2H3 3.98E+14 0.0 38808.0 T3XC6H9-1E34CH = P7XC7H10CH2C2H5 4.87E+14 0.0 42285.6 P6XC6H9-1E34CH = P1XCH2-2-HD 1.11E+12 0.0 15016.5 P6XC6H9-1E45CH = S3XC6H9-1E45CH 9.68E+11 0.0 17237.6 P6XC6H9-1E45CH = P8XC8H14-1E4C2H3 6.32E+13 0.0 30728.1 P6XC6H9-1E45CH = S4XC10H17-19E 5.08E+13 0.0 28188.4 S3XC6H9-1E45CH = P9XC9H14-13E5M 5.08E+13 0.0 28188.4 S3XC6H9-1E45CH = S9XC10H17-13E 1.44E+14 0.0 36596.3 P6XC6H9-1E45CH = P1XCH2-3-HD 2.03E+14 0.0 39358.5 S6XC6H9-1E56CH = S3XC6H9-1E56CH 3.70E+11 0.0 20299.3 S3XC6H9-1E56CH = C4H6 + cC6H11 7.08E+14 0.0 37532.2 S6XC6H9-1E56CH = cC6H10 + C4H7 9.61E+13 0.0 31620.3 S6XC6H9-1E56CH = P8XC8H14-1E5C2H3 4.24E+13 0.0 31207.0 S6XC6H9-1E56CH = P10XC10H17-15E 5.56E+13 0.0 30624.7 S6XC6H9-1E56CH = P1XCH2-2-HD 5.14E+10 0.0 7480.6 S6XcC10H17-1E = S3XcC10H17-1E 2.56E+12 0.0 30698.3 S6XcC10H17-1E = S4XcC10H17-1E 3.24E+12 0.0 37146.7 S6XcC10H17-1E = P10XC10H17-16E 2.47E+14 0.0 30267.0 S6XcC10H17-1E = P10XC10H17-17E 9.27E+13 0.0 29768.3 S3XcC10H17-1E = P10XC10H17-13E 3.13E+14 0.0 32498.7 S4XcC10H17-1E = P10XC10H17-14E 1.26E+14 0.0 26314.5 S4XcC10H17-1E = S1XC10H17-19E 1.90E+14 0.0 36963.9

!Decomposition and isomerization of alkenyl radicals

S9XC10H17-13E = S5XC10H17-13E 6.09E+10 0.0 9811.0 S9XC10H17-13E = S6XC10H17-13E 2.95E+11 0.0 23876.2 S5XC10H17-13E = C6H8-135E + pC4H9 1.21E+15 0.0 43634.9 S6XC10H17-13E = nC3H7 + C7H10-136E 6.79E+13 0.0 30376.3 S6XC10H17-13E = nC4H5 + C6H12-1E 1.20E+14 0.0 38307.3 S9XC10H17-13E = P7XC7H11-13E + C3H6 1.03E+14 0.0 30654.5 S9XC10H17-

13E = S1XC3H4CH3cC6H10 4.85E+09 0.0 2915.8 S4XC10H17-19E = S3XC10H17-19E 7.45E+10 0.0 11804.0 S4XC10H17-19E = C2H3 + C8H14-17E 4.96E+14 0.0 39116.0 S4XC10H17-19E = P5XC5H9-1E + C5H8-14E 1.11E+14 0.0 38863.7 S3XC10H17-19E = C4H6 + P6XC6H11-1E 4.42E+14 0.0 38774.2 S4XC10H17-19E = C3H5P1XCH2cC6H10 4.68E+09 0.0 6995.1 S1XC10H17-19E = S4XC10H17-19E 2.26E+12 0.0 16804.6 S1XC10H17-19E = S5XC10H17-19E 6.76E+11 0.0 9389.9 S1XC10H17-19E = C2H2 + P8XC8H15-1E 3.72E+13 0.0 35986.2 S5XC10H17-19E = aC3H5 + C7H12-16E 3.29E+13 0.0 12961.5 S5XC10H17-19E = C4H7 + C6H10-15E 9.02E+13 0.0 46117.0 S1XC10H17-16E = S4XC10H17-16E 3.24E+12 0.0 17429.9 S1XC10H17-16E = S5XC10H17-16E 6.73E+11 0.0 6522.8 S1XC10H17-16E = C2H2 + P1XC8H15-4E 1.62E+15 0.0 35308.6 S4XC10H17-16E = C2H3 + C8H14-14E 9.75E+13 0.0 38138.3 S4XC10H17-16E = C5H8-14E + S1XC5H9-1E 1.27E+14 0.0 38647.1 S5XC10H17-16E = aC3H5 + C7H12-13E 5.97E+13 0.0 28838.2 P10XC10H17-17E = S6XC10H17-17E 1.00E+12 0.0 15967.7 P10XC10H17-17E = C2H4 + S1XC8H13-17E 3.52E+14 0.0 38887.5 S6XC10H17-17E = C4H7 + C6H10-13E 3.82E+14 0.0 38315.2 P10XC10H17-16E = C2H4 + P8XC8H13-16E 5.35E+13 0.0 22193.1 P10XC10H17-16E = C5H9-1ES2XcC5H8 2.66E+11 0.0 15865.6 P10XC10H17-15E = S7XC10H17-15E 1.94E+12 0.0 20372.8 P10XC10H17-15E = P8XC8H13-15E + C2H4 5.31E+14 0.0 31759.4 S7XC10H17-15E = C8H12-137E + C2H5 3.21E+14 0.0 38446.4 P10XC10H17-15E = C4H7S2XcC6H10 8.12E+10 0.0 10012.9 P10XC10H17-15E = P1XC5H8-1EcC5H9 2.56E+11 0.0 7133.8 P10XC10H17-14E = S6XC10H17-14E 2.48E+16 0.0 19796.7 P10XC10H17-14E = S7XC10H17-14E 9.24E+16 0.0 31228.8 P10XC10H17-14E = P8XC8H13-14E + C2H4 2.03E+19 0.0 38498.0 S6XC10H17-14E = C7H10-136E + nC3H7 3.57E+14 0.0 38484.1 S7XC10H17-14E = C8H12-147E + C2H5 5.92E+13 0.0 30187.6 S7XC10H17-14E = S1XC5H7-14E + C5H10-1E 1.01E+14 0.0 52807.9 P10XC10H17-14E = S1XC4H6-3EcC6H11 3.44E+15 0.0 15217.4 P10XC10H17-13E = S6XC10H17-13E 8.20E+11 0.0 16815.3 P10XC10H17-13E = S7XC10H17-13E 2.38E+12 0.0 24017.3 P10XC10H17-13E = P8XC8H13-13E + C2H4 4.89E+14 0.0 32135.0 !S6XC10H17-13E = C6H12-1E + nC4H5 2.14E+14 0.0 38955.1 S7XC10H17-13E = C8H12-137E + C2H5 4.86E+13 0.0 30591.0 S7XC10H17-13E = P5XC5H7-13E + C5H10-1E 1.28E+13 0.0 19306.2 P9XC9H14-13E5M = S6XC9H14-13E5M 1.98E+12 0.0 24555.8 P9XC9H14-13E5M = T5XC9H14-13E5M 2.55E+11 0.0 9748.6 P9XC9H14-13E5M = P7XC7H10-13E5M + C2H4 3.32E+14 0.0 31165.3 S6XC9H14-13E5M = C6H12-2E + nC4H5 1.83E+14 0.0 38196.0 S6XC9H14-13E5M = C7H9-136E5M + C2H5 6.65E+13 0.0 30489.6 S6XC9H14-13E5M = C9H14-135E + CH3 2.80E+13 0.0 27558.5 T5XC9H14-13E5M = C6H7-135E2M + nC3H7 4.24E+14 0.0 42398.9 P9XC9H14-13E5M = S1XC3H4CH3cC6H10 9.74E+10 0.0 5928.0

P8XC8H14-3E4C2H3 = P6XC6H10-3E4C2H3 + C2H4 2.97E+14 0.0 30129.9 P8XC8H14-3E4C2H3 = S5XC8H14-3E4C2H3 1.41E+12 0.0 18215.9 S5XC8H14-3E4C2H3 = C6H9-13E-3-C2H3 + C2H5 1.91E+14 0.0 38706.7 P8XC8H14-3E4C2H3 = S1XC3H6C2H3cC5H8 2.97E+11 0.0 6946.5 P8XC8H14-

1E5C2H3 = S4XC8H14-1E5C2H3 2.82E+11 0.0 16426.0 P8XC8H14-1E5C2H3 = T5XC8H14-1E5C2H3 1.06E+12 0.0 17296.2 P8XC8H14-1E5C2H3 = P6XC6H10-1E5C2H3 + C2H4 9.06E+13 0.0 29134.3 S4XC8H14-1E5C2H3 = C6H11-1E-3-C2H3 + C2H3 1.06E+14 0.0 37695.2 S4XC8H14-1E5C2H3 = C7H10-136E + nC3H7 1.65E+13 0.0 25690.5 S4XC8H14-1E5C2H3 = C8H14-14E + C2H3 1.23E+14 0.0 36908.3

T5XC8H14-1E5C2H3 = C5H9-1E-2-C2H3 + aC3H5 6.80E+13 0.0 27731.4 T5XC8H14-1E5C2H3 = C6H9-15E-2-C2H3 + C2H5 9.78E+14 0.0 39920.9 P8XC8H14-1E5C2H3 = C4H7S2XcC6H10 5.98E+10 0.0 16024.4 P8XC8H14-1E4C2H3 = S5XC8H14-1E4C2H3 9.73E+11 0.0 22550.7 P8XC8H14-1E4C2H3 = T4XC8H14-1E4C2H3 1.21E+11 0.0 10797.8 P8XC8H14-1E4C2H3 = P6XC6H10-1E4C2H3 + C2H4 1.70E+14 0.0 30165.7 S5XC8H14-1E4C2H3 = C6H9-15E-3-C2H3 + C2H5 5.28E+13 0.0 29770.2 S5XC8H14-1E4C2H3 = C7H12-13E + aC3H5 4.88E+12 0.0 16753.1 S5XC8H14-1E4C2H3 = C8H14-14E + C2H3 7.78E+13 0.0 37806.5 T4XC8H14-1E4C2H3 = C6H8-15E-3-CH2 + nC3H7 1.42E+14 0.0 37496.5 T4XC8H14-1E4C2H3 = C7H12-1E-3-CH2 + C2H3 2.63E+15 0.0 48527.4 P7XC7H10CH2C2H5 = T4XC7H10CH2C2H5 1.57E+12 0.0 22312.3 P7XC7H10CH2C2H5 = P5XC5H61ECH2C2H5 + C2H4 8.33E+13 0.0 28878.0 T4XC7H10CH2C2H5 = C6H8-1E-34-CH2 + C2H5 1.19E+15 0.0 36308.1 T4XC7H10CH2C2H5 = C7H10-1E-34-CH2 + CH3 7.70E+14 0.0 40034.1 P7XC7H10CH2C2H5 = C2H5C2H3S2XcC6H9 8.42E+10 0.0 6452.0 P1XC10H17-46E = T4XC10H17-46E 3.09E+12 0.0 21708.2 P1XC10H17-46E = P1XC8H13-24E + C2H4 4.41E+13 0.0 13179.3 T4XC10H17-46E = S1XC5H9-1E + C5H8 2.41E+16 0.0 41371.5 P1XC10H17-46E = S1XC4H8cC6H9-2E 1.96E+11 0.0 6779.9 P1XC9H15-3E5CH2 = T4XC9H15-3E5CH2 5.19E+12 0.0 25811.7 P1XC9H15-3E5CH2 = S1XC7H11-1E3CH2 + C2H4 1.06E+15 0.0 38923.3 T4XC9H15-3E5CH2 = C2H5 + C7H10-3-CH2 7.18E+14 0.0 39513.5 P1XC9H15-3E5CH2 = C4H9T1XcC6H8-2E 2.84E+11 0.0 8909.2 P1XC8H13-45-CH2 = S1XC6H9-23-CH2 + C2H4 3.30E+13 0.0 21897.0 P1XC8H13-45-CH2 = C5H9-1EcC5H8 3.47E+11 0.0 11091.4 P1XC8H13-45-CH2 = C3H7CH2T1XcC6H8 3.16E+11 0.0 10498.6

!Dissociation of alkenecyclohexane

C6H10-1E56CH + H = S3XC6H9-1E56CH + H2 2.42E+14 0.0 8169.8 C6H10-1E56CH = PXCH2cC6H11 + aC3H5 2.78E+15 0.0 67413.8 C6H10-1E45CH + H = S3XC6H9-1E45CH + H2 1.77E+14 0.0 7933.3 C6H10-1E45CH = S2XMCH + aC3H5 1.86E+15 0.0 64097.1 C6H10-1E34CH + H = T3XC6H9-1E34CH + H2 1.68E+14 0.0 9175.9

!Stepwize dehydrogenation of cyclic intermediate methylhydrindane

spiro-4-5-decane + H = S1Xspiro-4-5-DN + H2 2.75E+14 0.0 11058.0 P1XCH2-1-HD = S8XHD-1M 2.26E+13 0.0 23437.0 S8XHD-1M = HD-7E1M + H 1.93E+14 0.0 36936.1 HD-7E1M + H = S6XHD-7E1M + H2 2.84E+14 0.0 8837.9 S6XHD-7E1M = HD-57E1M + H 4.15E+14 0.0 45783.1

HD-57E1M + H = S4XHD-57E1M + H2 3.59E+14 0.0 7734.8 S4XHD-57E1M = HD-357E1M + H 7.78E+13 0.0 52450.2 HD-357E1M + H = S2XHD-357E1M + H2 2.32E+14 0.0 9973.6 S2XHD-357E1M = indene + CH3 1.56E+15 0.0 45224.7 P1XCH2-2-HD = S4XHD2M 2.30E+12 0.0 35566.9 S4XHD2M = HD-4E2M + H 7.30E+13 0.0 35765.6 HD-4E2M + H = T1XHD-4E2M + H2 1.21E+14 0.0 5798.5 T1XHD-4E2M = HD-14E + CH3 9.64E+14 0.0 41441.1 HD-14E + H = S6XHD-14E + H2 3.33E+14 0.0 9622.6 S6XHD-14E = HD-146E + H 7.38E+14 0.0 49201.1 HD-146E + H = S8XHD-146E + H2 3.51E+14 0.0 9834.1 S8XHD-146E = indene + H 4.47E+14 0.0 46321.6 P1XCH2-3-HD = T1XHD3M 3.79E+12 0.0 23085.3 T1XHD3M = HD-1bE3M + H 1.27E+14 0.0 35332.4 HD-1bE3M + H = S2XHD-1bE3M + H2 1.21E+14 0.0 7462.1 S2XHD-1bE3M = HD-1b2E + CH3 7.85E+14 0.0 40620.4 HD-1b2E + H = S6XHD-1b2E + H2 3.28E+14 0.0 6565.7 S6XHD-1b2E = HD-1b26E + H 1.08E+14 0.0 55401.1 HD-1b26E + H = S7XHD-1b26E + H2 4.31E+14 0.0 5745.6 S7XHD-1b26E = indene + H 1.35E+14 0.0 33430.7

!Cyclohexane

C2H5C2H3S2XcC6H9 = C2H3cC6H9 + C2H5 1.38E+15 0.0 37399.1 C3H7CH2T1XcC6H8 = CH2-12-cC6H8 + C2H5 9.31E+14 0.0 40678.0 CH2-12-cC6H8 = CH2-2-CH3cC6H7 4.51E+13 0.0 94441.7 CH2-2-CH3cC6H7 = DCH-15E 4.92E+13 0.0 93887.3 DCH-15E + H = S3XDCH-15E + H2 7.58E+14 0.0 6472.5 S3XDCH-15E = o-xylene + H 1.26E+14 0.0 30358.5 C4H7S2XcC6H10 = cC6H10 + C4H7 2.88E+14 0.0 31825.0 C4H9T1XcC6H8-2E = CH2cC6H8-2E + nC3H7 8.92E+14 0.0 39052.5 CH2cC6H8-2E = MCH-15E 2.72E+13 0.0 94698.0 !MCH-15E + H = S3XMCH-15E + H2 3.76E+14 0.0 6363.4 S3XMCH-15E = A1CH3 + H 5.01E+13 0.0 31612.4 S1XC3H4CH3cC6H10 = C3H5CH3S6XcC6H10 1.11E+13 0.0 58294.5 C3H5CH3S6XcC6H10 = MCH-2E + aC3H5 2.12E+13 0.0 22687.9 !MCH-2E + H = T1XMCH-2E + H2 1.72E+14 0.0 5798.6 T1XMCH-2E = MCH-15E + H 3.18E+14 0.0 51241.9 S1XC3H4CH3cC6H10 = C3H5P1XCH2cC6H10 9.60E+13 0.0 49976.1 C3H5P1XCH2cC6H10 = C3H5CH3S3XcC6H9 1.77E+13 0.0 39930.8 C3H5CH3S3XcC6H9 = C3H5CH3cC6H8-2E + H 1.89E+14 0.0 39008.7 C3H5CH3cC6H8-2E + H = C3H5CH3S4XcC6H8 + H2 3.11E+14 0.0 9022.7 C3H5CH3S4XcC6H8 = C3H5CH3cC6H8-24E + H 7.39E+14 0.0 51490.3 C3H5CH3cC6H8-24E + H = C3H5CH3S6XcC6H8 + H2 2.46E+14 0.0 6644.2 C3H5CH3S6XcC6H8 = A1CH3 + aC3H5 2.29E+13 0.0 13541.4 S1XC4H6-3EcC6H11 = C2H3cC6H11 + C2H3 3.85E+14 0.0 37301.7 C2H3cC6H11 + H = C2H3T1XcC6H10 + H2 8.80E+13 0.0 7117.6 C2H3T1XcC6H10 = C2H3cC6H9 + H 1.63E+15 0.0 49666.1 S1XC4H8cC6H9 = C2H3cC6H9 + C2H5 8.51E+14 0.0 39807.6 C2H3cC6H9 + H = CH2CH-1-SAXcC6H8 + H2 3.69E+14 0.0 6372.4 CH2CH-1-SAXcC6H8 = CH2CH-1-cC6H7-13 + H 1.77E+15 0.0 57068.4 !CH2CH-1-cC6H7-13 + H = CH2CH-1-SAXcC6H6 + H2 3.20E+14 0.0 7980.2 CH2CH-1-SAXcC6H6 = A1C2H3 + H 1.14E+14 0.0 33394.9 S1XC4H8cC6H9-2E = C2H3cC6H9-2E + C2H5 1.37E+14 0.0 29851.7 C2H3cC6H9-2E + H = C2H3T1XcC6H8-2E + H2 1.60E+14 0.0 6701.0 C2H3T1XcC6H8-2E = CH2CH-2-cC6H7-13

+ H 2.73E+14 0.0 60021.4 !CH2CH-2-cC6H7-13 + H = CH2CH-3-SAXcC6H6 + H2 4.13E+14 0.0 5963.8 CH2CH-3-SAXcC6H6 = A1C2H3 + H 3.69E+14 0.0 35674.2

!cyclopentane

C5H9-1EcC5H8 = C5H9-1EcC5H7 + H 1.04E+14 0.0 44743.8 C5H9-1EcC5H7 + H = C5H9-1EcC5H6 + H2 2.23E+14 0.0 6026.0 C5H9-1EcC5H6 = C5H9-1EcC5H5 + H 6.59E+13 0.0 51625.5 C5H9-1EcC5H5 = T1XcC5H5 + T2XC5H9-1E 9.68E+16 0.0 110122.7 C5H9-1ES2XcC5H8 = cC5H8 + S1XC5H9-1E 4.50E+14 0.0 37876.0 P1XC5H8-1EcC5H9 = C2H3cC5H9 + aC3H5 2.29E+13 0.0 20505.9 C2H3cC5H9+ H = C2H3T1XcC5H8 + H2 8.10E+13 0.0 8904.0 C2H3T1XcC5H8 = C2H3cC5H7 + H 1.65E+14 0.0 47269.5 C2H3cC5H7 + H = C2H3S3XcC5H6 + H2 2.80E+14 0.0 7309.5 C2H3S3XcC5H6 = C2H3cC5H5 + H 1.40E+14 0.0 53000.6 C2H3cC5H5 = T1XcC5H5 + C2H3 1.15E+17 0.0 113540.7 !P1XCH2-C4H9-cC5H6-2E = CH2cC5H6 + pC4H9 1.69E+14 0.0 27236.6 !CH2cC5H6 = cC5H5-13E2M 1.54E+13 0.0 83933.4 S1XC3H6C2H3cC5H8 = C2H3C2H3cC5H8 + CH3 8.43E+13 0.0 31342.1 C2H3C2H3cC5H8 + H = C2H3C2H3S2XcC5H8 + H2 2.80E+14 0.0 13284.4 C2H3C2H3S2XcC5H8 = C2H3cC5H7 + C2H3 3.45E+14 0.0 33255.8

!olefinic decalin

decalin-1bE + H = S2Xdecalin-1bE + H2 1.12E+15 0.0 6679.8 S2Xdecalin-1bE = decalin-1b2E+H 8.59E+14 0.0 50459.0 decalin-1b2E + H = S4Xdecalin-1b2E + H2 3.79E+14 0.0 6370.2 S4Xdecalin-1b2E = tetralin+H 1.56E+14 0.0 31290.5 tetralin + H = S7Xdecalin-1b24E + H2 6.25E+14 0.0 10109.7 S7Xdecalin-1b24E = decalin-1b247E+H 5.95E+14 0.0 46242.1 decalin-1b247E + H = S9Xdecalin1b247E + H2 3.54E+14 0.0 10943.7 S9Xdecalin1b247E = naphthalene+H 1.40E+14 0.0 34815.7 decalin-1bE = C2H4 + CH2-12-cC6H8 1.43E+15 0.0 67296.5 decalin-1E + H = T6Xdecalin-1E + H2 1.66E+14 0.0 5494.0 T6Xdecalin-1E = decalin-15E+H 1.76E+14 0.0 51432.7 decalin-15E + H = S3Xdecalin-15E + H2 8.24E+14 0.0 10771.6 S3Xdecalin-15E = tetralin+H 1.31E+14 0.0 30447.9 decalin-1E = C2H4 + C2H3cC6H9 4.60E+15 0.0 68697.5 decalin-2E + H = T1Xdecalin-2E + H2 1.24E+14 0.0 5889.9 T1Xdecalin-2E = decalin-1b2E+H 1.67E+14 0.0 48555.2 decalin-3E + H = S2Xdecalin-3E + H2 4.56E+14 0.0 7499.7 S2Xdecalin-3E = decalin-13E+H 9.29E+13 0.0 48692.4 decalin-13E + H = T6Xdecalin-13E + H2 8.51E+14 0.0 4097.4 T6Xdecalin-13E = tetralin+H 1.56E+14 0.0 31290.5 decalin-3E = C4H6 + cC6H10 1.64E+15 0.0 69561.9

HYD-RXN-STARTS-HERE

!Unimolecular decomposition (C-H bond dissociation) HYD = T1X-HYD+H 9.54E+14 0.00 97682.9 HYD = S2X-HYD+H 1.70E+16 0.00 103196.8 HYD = S3X-HYD+H 1.78E+16 0.00

101835.7 HYD = S7X-HYD+H 6.35E+15 0.00 101356.9 HYD = S8X-HYD+H 2.85E+15 0.00 99977.9

!Ring opening isomerization (C-C bond dissociation) HYD = INT1A 8.00E+16 0.00 91631.8 HYD = INT2B 1.06E+17 0.00 96430.9 HYD = INT3C 1.70E+17 0.00 95222.6 HYD = INT4D 6.96E+15 0.00 84517.6 HYD = INT5E 3.84E+15 0.00 88007.1

!Ring opening isomerization (H-migration) INT1A = C4H71EcC5H9 4.49E+11 0.00 9834.9 INT2B = CH3C3H51EcC5H8 5.30E+11 0.00 6272.8 INT2B = CH21EC3H7cC5H7 5.37E+10 0.00 5436.0 INT3C = C2H5C2H31EcC5H8 3.50E+11 0.00 7079.2 INT4D = C3H51EcC6H11 3.83E+12 0.00 16104.3 INT5E = CH3C2H31EcC6H10 1.51E+12 0.00 10874.6 INT5E = CH2C2H51EcC6H9 2.12E+12 0.00 22693.8

!Dissociation of alkene cyclopentane taken from decalin (CHECK ALL AGAIN)

C4H71EcC5H9+H=C4H71ES2XcC5H8+H2 1.68E+14 0.0 9175.9 C4H71EcC5H9=cC5H9+C4H7 2.78E+15 0.0 67413.8

CH3C3H51EcC5H8+H=CH2C3H51EcC5H8+H2 2.42E+14 0.0 8169.8 CH3C3H51EcC5H8=CH3S2XcC5H8 +aC3H5 2.78E+15 0.0 67413.8

CH21EC3H7cC5H7+H=CH2P1XC4H8cC5H7+H2 2.42E+14 0.0 8169.8

CH21EC3H7cC5H7=nC3H7+CH2S2XcC5H7 2.78E+15 0.0 67413.8 CH2S2XcC5H7=C2H3-2-PXC4H6 3.47E+10 0.959 33910 ! HPL, 2-methylcyclopentyl radical decomposition, 2008 Sirjean et al. !J. Phys. Chem. A 112 (2008) 11598-1161 !(ALREADY PRESENT)C2H3-2-PXC4H6=iC4H5+C2H5

!C2H5C2H31EcC5H8 ADD REACTIONS C2H5C2H31EcC5H8+H=C2H4C2H31EcC5H8+H2 2.42E+14 0.0 8169.8 C2H5C2H31EcC5H8=C2H5+C2H3S2XcC5H8 2.78E+15 0.0 67413.8

!Dissociation of alkene cyclohexane taken from decalin (CHECK ALL AGAIN)

C3H51EcC6H11+H=C3H61ES1XcC6H10+H2 1.68E+14 0.0 9175.9

CH3C2H31EcC6H10+H=CH2C2H31EcC6H10+H2 2.42E+14 0.0 8169.8 CH3C2H31EcC6H10=CH2CH-2-cC6H10+CH3 4.34E+14 0.0 39489.6 !S3XcC5H64M = C5H6+CH3

CH2C2H51EcC6H9+H=C2H4CH21EcC6H9+H2 2.42E+14 0.0 8169.8 !C2H4CH21EcC6H9= already done in radical dissociation !already done in radical dissociation CH2C2H51EcC6H9=CH2S2XcC6H9+C2H5

C3H51EcC6H11=cC6H11+aC3H5 2.78E+15 0.0 67413.8

! CH3-abstractions of hyd

HYD+CH3 = T1X-HYD+CH4 7.05E+12 0.00 14879.8 HYD+CH3 = S2X-HYD+CH4 5.85E+13 0.00 17732.8 HYD+CH3 = S3X-HYD+CH4 7.07E+13 0.00 18037.2 HYD+CH3 = S7X-HYD+CH4 2.52E+13 0.00 17779.7 HYD+CH3 = S8X-HYD+CH4 1.30E+13 0.00 16879.7

! H-abstractions of HYD 0.00 HYD+H = T1X-HYD+H2 2.44E+14 0.00 8033.9 HYD+H = S2X-HYD+H2 6.44E+14 0.00 11115.6 HYD+H = S3X-HYD+H2 6.77E+14 0.00 11326.1 HYD+H = S7X-HYD+H2 4.07E+14 0.00 11027.0 HYD+H = S8X-HYD+H2 1.80E+14 0.00 10002.8

! hydrindane radicals- H elimination T1X-HYD = HYD-6E +H 2.59E+14 0.00 37518.3 T1X-HYD = HYD-16E+H 2.51E+14 0.00 36535.6 T1X-HYD = HYD-5E+H 1.50E+14 0.00 34652.8 S2X-HYD = HYD-1E +H 4.54E+13 0.00 35509.3 S2X-HYD = HYD-2E +H 1.42E+14 0.00 37583.9 S3X-HYD = HYD-3E +H 2.03E+14 0.00 38154.2 S3X-HYD = HYD-2E +H 1.64E+14 0.00 36387.6 S7X-HYD = HYD-7E +H 2.30E+14 0.00 39523.4 S7X-HYD = HYD-6E +H 7.17E+13 0.00 35473.5 S8X-HYD = HYD-7E +H 1.00E+14 0.00 41059.5

! decomposition and isomerization of T1X RADICAL(good)

T1X-HYD =CH2P1XC4H8cC5H7 1.23E+14 0.00 33585.7 CH2P1XC4H8cC5H7=CH2ECH2cC5H7+C2H4 7.54E+12 0.00 28168.6

! ADD RATES CH2ECH2cC5H7=P1XC3H6C4H513E 5.87E+13 0.00 35433.8 P1XC3H6C4H513E=P1XCH2C4H 13E+C2H4 2.38E+13 0.00 18788.0 CH2ECH2cC5H7=T2XC7H11-16E 5.19E+13 0.00 31115.6

T1X-HYD=C2H4CH21EcC6H9 3.68E+13 0.00 38247.6 C2H4CH21EcC6H9=CH2S2XcC6H9+C2H4 1.13E+14 0.00 24549.4

!already there CH2S2XcC6H9=CH2cC6H8-2E+H 1.82E+20 -3.68 23447 ! CH2S2XcC6H9=CH2cC6H8-2E+H

T1X-HYD = P1XC3H6cC6H9 1.22E+14 0.00 35584.7904 P1XC3H6cC6H9=P1XCH2-1-cC6H9+C2H4 3.18E+13 0.00 21213.36

P1XCH2-1-cC6H9+H=MCH-1E 4.0E+14 0.00 0.0 !S2XMCH=cC6H10+CH3 cC6H9+H=cC6H10 4.0E+14 0.00 0.0 !CH2S2XcC6H9+H(+M)=CH2cC6H10(+M)

T1X-HYD=P1XC4H8cC5H71E 1.55E+14 0.00 31963.8 P1XC4H8cC5H71E=P1XC2H4cC5H71E+C2H4 1.39E+14 0.00 28941.6 P1XC2H4cC5H71E=cC5H71-2+C2H4 1.84E+15 0.00 40423.6

!decomposition and isomerization of S7X(GOOD)

S7X-HYD = S5XcC9H151E 5.03E+13 0.00 34756.6 S5XcC9H151E = S9XC9H1517E 1.04E+14 0.00 33069.0 S9XC9H1515E =C2H4+S7XC7H11-15E 1.48262E+14 0.00 29744.4096

S5XcC9H151E = S9XC9H1515E 6.16E+13 0.00 24973.1

S7X-HYD = CH2C2H31EcC6H10 4.24E+13 0.00 35193.3 CH2C2H31EcC6H10 =S3XC9H1518E 1.65E+13 0.00 19899.8 S3XC9H1518E=P5XC5H9-1E+C4H6 1.06E+15 0.00 38504.0 !P5XC5H9-1E = aC3H5+C2H4 1.67E+13 0.00 20708.6 NO NEED

CH2C2H31EcC6H10=P7XC4H8C5H714E 4.34E+13 0.00 30137.9 S7X-HYD = P1XC4H8cC5H7-2E 5.76E+13 0.00 37238.1 P1XC4H8cC5H7-2E=P1XC2H4cC5H72E+C2H4 1.76E+14 0.00 29835.8 P1XC2H4cC5H72E=cC5H71-3+C2H4 3.72E+13 0.00 20295.3

P7XC4H8C5H714E= P5XC2H4C5H714E+C2H4 2.38169E+14 0.0 29623.2 P5XC2H4C5H714E=S3XC5H7-14E+C2H4 1.55E+13 0.00 14327.3 S3XC5H7-14E+H=C5H8-14E 8.48E+11 0.51 1230 ! TAKEN FROM cp

! decomposition and isomerization of S8X RADICAL(good)

S8X-HYD=C3H61ES1XcC6H10 4.33E+13 0.00 35358.2 C3H61ES1XcC6H10 = P1XC3H6C6H915E 5.96E+13 0.00 31145.4 P1XC3H6C6H915E = P1XCH2C6H915E+C2H4 7.34E+13 0.00 28313.6 P1XCH2C6H915E = C4H6+aC3H5 4.60E+13 0.00 18826.3 P1XCH2C6H915E = C5H8-14E+C2H3 3.71E+14 0.00 36439.3

C3H61ES1XcC6H10= S9XC9H1514E 6.93E+13 0.00 30529.4 S9XC9H1514E = S7XC7H11-14E+C2H4 1.48E+14 0.00 29744.4 S7XC7H11-14E = T1XC5H7-14E+C2H4 1.20E+15 0.00 38615.3

C3H61ES1XcC6H10= aC3H5+cC6H10 6.35E+13 0.00 23896.1

! decomposition and isomerization of S3X RADICAL

S3X-HYD = C4H71ES2XcC5H8 5.83E+13 0.00 33287.6 C4H71ES2XcC5H8 = P9XC9H1515E 1.18E+14 0.00 32657.6 P9XC9H1515E=P7XC7H11-15E + C2H4 1.48E+14 0.00 29744.4 P7XC7H11-15E= C4H6+aC3H5 3.39E+11 0.66 32262.9 ! Ref to S3XC6H11-1E(+M) = C4H6+C2H5(+M) ! LOW / 4.00E-42 18.05-602.6 / ! TROE /-18.50 246 28 50000.0 / ! H2/2/ CH4/2/ C2H6/3/ AR/0.7/ !C7H12-15E+H = S3XC7H11-15E+H2 3.376E5 2.36 207 ! allyls LLNL-MI 407571 !C7H12-15E+H = S4XC7H11-15E+H2 3.376E5 2.36 207 ! allyls LLNL-MI 407571 !C7H12-15E+CH3 = S3XC7H11-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI 407571 !C7H12-15E+CH3 = S4XC7H11-15E+CH4 3.69 3.31 4002 ! allyls LLNL-MI 407571 !C7H12-15E+H= P7XC7H11-15E+H2 1.7298E5 2.5 2492 ! allylP LLNL-MI 407571 !C7H12-15E+CH3 = P7XC7H11-15E+CH4 2.2098 3.5 5675 ! allylP LLNL-MI 407571 C4H71ES2XcC5H8 = C4H7+cC5H8 4.41E+14 0.00 29476.1 C4H71ES2XcC5H8=P1XC2H4C7 7.53E+13 0.00 32361.6 P1XC2H4C7H1216E=S3XC7H11-16E + C2H4 2.38E+13 0.00 18787.9

S3X-HYD =CH2C3H51EcC5H8 1.24E+14 0.00 30410.1 CH2C3H51EcC5H8 = S4XC9H1518E 3.77E+12 0.00 21133.9 S4XC9H1518E=C7H12-16E+C2H3 1.48E+14 0.00 29744.4096 ! S9XC9H1515E =C2H4+S7XC7H11-15E S4XC9H1518E=C5H8-14E+C4H7 1.06E+15 0.00 38504.0 ! S3XC9H1518E=P5XC5H9-1E+C4H6

CH2C3H51EcC5H8 = P1XC3H6C6H915E 5.72E+12 0.00 23091.3 P1XC3H6C6H915E=P1XCH2-3C6H9-15E+C2H4 7.3404E+13 0.0 28313.6256 P1XCH2-3C6H9-15E=C5H8-14E+C2H3 3.71288E+14 0.0 36439.2864 P1XCH2-3C6H9-15E=C4H6+aC3H5 4.59695E+13 0.0 18826.33536

!P1XC2H4C7H1216E=S3XC7H11-16E+C2H4 2.38E+13 0.00 18788.0 !S3XC7H11-16E=aC3H5 +C4H6 1.20E+14 0.00 28587.9 ALREADY THERE

! decomposition and isomerization of S2X(GOOD)

S2X-HYD = P1XC3H6cC6H9 6.50E+13 0.00 33043.2 P1XC3H6cC6H9=P1XCH2-2-cC6H9+C2H4 8.90E+12 0.00 22834.9

!******* ADD THIS H elimination (ALREADY ADDED) !P1XCH2-2-cC6H9=CH2cC6H8-2E+H 4.41E+14 0.00 2476.1 !

S2X-HYD = S5XcC9H155E 1.67E+13 0.00 27079.6 S5XcC9H155E=P9XC9H1516E 1.16E+14 0.00 28291.8 P9XC9H1516E= T1XC7H11-16E+C2H4 1.48E+14 0.00 29744.4096 !T1XC7H11-16E+H= C7H11-16E(PRESENT)+H2

S2X-HYD = C2H4C2H31EcC5H8 9.99E+13 0.00 30352.5 C2H4C2H31EcC5H8 = C2H3S2XcC5H8+C2H4 4.94E+13 0.00 26640.4 !C2H3S2XcC5H8=cC5H8+C2H3 6.75E+14 0.00 37949.6 already added by subharaj !C2H3S2XcC5H8= P1XC2H4C3H714E 5.87E+13 0.00 35433.8 !C2H3S2XcC5H8 = P7XC7H1113E 5.19E+13 0.00 31115.6

!Hydrindene reactions

!HYD-1E

HYD-1E+H=T6X-HYD-1E+H2 1.72E+14 0.00 5485.9 T6X-HYD-1E=C2H4CH21EcC6H7 5.50E+13 0.00 45264.4

! CHECK BOTH C2H4CH21EcC6H7=CH21ES2XcC6H71E+C2H4 1.13E+14 0.00 24549.4 !C2H4CH21EcC6H9=CH21ES2XcC6H71E+H=CH2cC6H8-2E 1.72E+14 0.00 5485.9 !HYD-1E+H=T6X-HYD-1E+H2

T6X-HYD-1E=C3H5CH21EcC5H6 1.69E+14 0.00 43823.7 C3H5CH21EcC5H6=CH21ECH21EcC5H6+C2H4 1.61E+13 0.00 20704.6

!HYD-2E

HYD-2E+H=T1X-HYD-2E+H2 1.39E+14 0.00 5456.9 T1X-HYD-2E=P1XC3H6cC6H715E 6.84E+13 0.00 44052.2 P1XC3H6cC6H715E=P1XMCH-15E+C2H4 2.05E+14 0.00 30555.2 T1X-HYD-2E=P1XC4H63EcC5H7 2.09E+14 0.00 39479.7 P1XC4H63EcC5H71E=P1XC2H21EcC5H71E+C2H4 2.47E+14 0.00 30583.0 P1XC2H21EcC5H71E+H=C2H3cC5H7 4.41E+14 0.00 2476.1 !

CH21EC2H4cC6H73E=CH2S2XcC6H7-5E+C2H4 9.07E+14 0.00 41186.7 CH2S2XcC6H7-5E=CH2cC6H6-25E+H 1.72E+14 0.00 45485.9 !H-ELIMINATION-CHECK

T1X-HYD-2E=CH21EC2H4cC6H73E 1.46E+14 0.00 40012.3

!HYD-7E HYD-7E+H=T1X-HYD-7E+H2 1.63E+14 0.00 5466.6 T1X-HYD-7E=P1XC3H4EcC6H9E 2.25E+14 0.00 45111.4 T1X-HYD-7E=C3H6CH2EcC5H5E 1.80E+14 0.00 44312.6 C3H6CH2EcC5H5E=CH2CH21E 2E+C2H4 3.98E+13 0.00 20124.4 T1X-HYD-7E=P1XC4H8cC5H514E 2.90E+14 0.00 43636.9 P1XC4H8cC5H514E= 5.82E+14 0.00 37375.3 P1XC2H4cC5H514E=C5H5+C2H4 6.62E+13 0.00 22622.3

!CH2CH21EcC5H5-2E=CH2S2XC5H5+CH3 4.24E+21 -3.89 22867 !S2XMCH=cC6H10+CH3 !C5H5CH2-2+H=FULVENE 4.94E+18 -1.28 5411 !Ahren W. Jasper 2013

!HYD-6E HYD-6E+H=T1X-HYD-6E+H2 1.83E+14 0.00 4676.9 T1X-HYD-6E=P1XC2H3CH2cC6H9 7.95E+13 0.00 45882.5 P1XC2H3CH2cC6H9=CH21ES2XcC6H71E+C2H4 4.10E+14 0.00 36067.7 T1X-HYD-6E=P1XC3H6CH2cC5H5 1.81E+14 0.00 46530.3 P1XC3H6CH2cC5H5=CH2CH21EcC5H51E+C2H4 5.28E+13 0.00 36375.7

!HYD-16E HYD-16E+H=S6X-HYD-16E+H2 2.85E+14 0.00 8406.3 HYD-16E+H=S2X-HYD-16E+H2 2.67E+14 0.00 6988.2 S2X-HYD-16E=P1XCH2C2H3cC6H8 7.09E+13 0.00 44076.1 P1XCH2C2H3cC6H8= 5.41E+14 0.00 40111.632 C2H3T2XcC5H6+H=C2H3cC5H7 4.41E+14 0.00 2476.1 ! S6X-HYD-16E=PXC2H4C2H3cC5H6 2.28E+14 0.00 43633.0 PXC2H4C2H3cC5H6=S1XC2H3cC5H6-1E+C2H4 5.41E+14 0.00 39811.6

END

A.2 Reaction mechanism of methyl cyclopentane

ELEMENTS C H N O AR HE END SPECIES INTa INTb INTc INT1 INT2 INT3 AR N2 HE H2 H O2 O H2O OH OHV H2O2 HO2

CO CO2 HOCO CH4 CH3 CH2 CH2(S) C CH CHV CH3O2H CH3O2 CH2O2H CH3OH CH3O CH2OH CH2O HCO HCOH HO2CHO HOCH2O2H HOCH2O2 OCH2O2H HOCH2O O2CHO HOCHO OCHO

C2H6 C2H5 C2H5O2H C2H5O2 C2H4 C2H3 CHOCHO C2H3OOH C2H3OO CHCHO C2H2 C2H H2CC C2H5OH C2H5O PC2H4OH SC2H4OH O2C2H4OH C2H4O2H C2H4O1-2 C2H3O1-2 CH3CHO CH3CO CH2CHO O2CH2CHO HO2CH2CO C2H3OH C2H2OH CH2CO HCCO HCCOH CH3CO3H CH3CO3 CH3CO2 CH3OCH3 CH3OCH2 CH3OCH2O2H CH3OCH2O2 CH2OCH2O2H O2CH2OCH2O2H HO2CH2OCHO OCH2OCHO HOCH2OCO CH3OCH2O CH3OCHO CH3OCO CH2OCHO

C3H8 IC3H7 NC3H7 NC3H7O2H NC3H7O2 IC3H7O2H IC3H7O2 NC3H7O IC3H7O C3H6OOH1-2 C3H6OOH1-3 C3H6OOH2-1 C3H6OOH1-2O2 C3H6OOH1-3O2 C3H6OOH2-1O2 C3KET12 C3KET13 C3H51-2,3OOH C3H52-1,3OOH C3H5O1-2OOH-3 C3H5O1-3OOH-2 C3H6O1-2 C3H6O1-3 C3H6 C3H5-A C3H5-S C3H5-T CC3H6 C3H5O CH2CHOCH2 CH3CHCHO AC4H7OOH C3H6OH1-2 CH3CHCO AC3H5OOH C3H6OH2-1 HOC3H6O2 SC3H5OH IC3H5OH C3H5OH CH2CCH2OH C3H4-P C3H4-A C3H3 CC3H4 C3H2 H2CCC(S) C3H2(S) C3H2C PC3H4OH-2 SC3H4OH C3H3O C3H3O2H C2HCHO C2H5CHO C2H5CO CH2CH2CHO C2H3CHO C2H3CO CH3COCH3 CH3COCH2 CH3COCH2O2 CH3COCH2O C3KET21

C4H10 PC4H9 SC4H9 PC4H9O SC4H9O PC4H9O2 SC4H9O2 PC4H9O2H SC4H9O2H C4H8OOH1-2 C4H8OOH1-3 C4H8OOH1-4 C4H8OOH2-1 C4H8OOH2-3 C4H8OOH2-4 C4H8O1-2 C4H8O1-3 C4H8O1-4 C4H8O2-3 C4H8OOH1-2O2 C4H8OOH1-3O2 C4H8OOH1-4O2 C4H8OOH2-1O2 C4H8OOH2-3O2 C4H8OOH2-4O2 C4H71-2,4OOH C4H72-1,3OOH C4H72-1,4OOH C4H71-2,3OOH C4H7O1-3OOH-4 C4H7O1-3OOH-2 C4H7O1-2OOH-4 C4H7O1-4OOH-2 C4H7O1-2OOH-3 C4H7O2-3OOH-1 C4H72-1OOH NC4KET12 NC4KET13 NC4KET14 NC4KET21 NC4KET23 NC4KET24 C4H71-3OOH C4H71-3,4OOH C4H72-3,4OOH HO2CH2CHO IC4H10 IC4H9 TC4H9 TC4H9O IC4H9O IC4H8O IC3H7CHO IC3H7CO IC3H6CHO TC3H6CHO IC3H5CHO TC3H6O2CHO IC3H5O2HCHO TC3H6O2HCO TC3H6OCHO IC3H6CO IC3H5CO IC3H4CHO-A SC4H7OH-I IC4H9O2 TC4H9O2 IC4H8O2H-I IC4H8O2H-T TC4H8O2H-I CC4H8O IC4H8OOH-IO2 IC4H8OOH-TO2 TC4H8OOH-IO2 IC4KETII IC4KETIT TIC4H7Q2-I IIC4H7Q2-I IIC4H7Q2-T IC4H7OOH IC4H9O2H TC4H9O2H IC4H8 IC4H7 IC4H7-I1 IC4H7O2 IC4H6OOH-I CCYCCOOC-T1 C2CYCOOC-I1 IC4H7O CVCYC-COC CCYC2OCO CCYCCOOC-I2 CHOIC3H6O IC3H5OOCH2 IC4H8OH-IT IC4H8OH-TI IC4H7OH IC4H8OH IC4H6OH TQJC4H8OH TQC4H8OI QC4H7OHP TQC4H7OHI CCY(CCO)COH C2CY(COC)OH IQJC4H8OH IC3H6OHCHO IQC4H8OT IQC4H7OHT CCY(CCOC)OH CH2COHCH2OOH TC3H6OH TQC4H7OHIO2 TQC4H7OHTO2 TQC4H7OHIQ-I TQC4H7OHIQ-P IC3H5COHQ CH2CQCOHQ IC3H5Q COHQCYC(COC) QCYC(CCOC)OH HOCOCQ(CH3)2 IQC4H7OHTO2 IQC4H8OTQ-I IQC4H7OHTQ-

P CHOC(CH3)OHCH2Q CO(CH2OOH)2 IC3H5OCH2 IC4H7OOCH3 IC4H7OOIC4H7 C4H8-1 C4H8-2 C4H71-1 C4H71-2 C4H71-3 C4H71-4 C4H72-2 C4H71-O PC4H8OH-2 SC4H8OH-1 SC4H8OH-3 C4H71-3OH C4H71-4OH C4H71-1OH C4H71-2OH C4H72-1OH C4H72-2OH SQC4H8OP PQC4H8OS PQC4H7OHS-3 NC4KET12OH SQC4H7OHS-4 SQC4H8OS NC4KET23OH SC4H8OH-3O2 CCY(COCC)OH C4H7O2-1 C4H6-1 AC3H5OCH2 SC3H5OCH2-1 C8H141-5,3-4 C8H141-5,3 C8H142-6 C8H131-5,3-4,TA C8H131-5,3,TA C8H131-5,3,SA C8H131-5,3,PA C8H132-6,SA C8H132-6,PA C6H101-3,3 C8H131-5,3-4,TAO C8H131-5,3,TAO C8H131-5,3,SAO C8H131-5,3,PAO C8H132-6,SAO C8H132-6,PAO C7H111-5,3,6P C7H111-5,1P C4H64,2-1OH C4H63,1-1OH C4H63,1-3OH C4H63,1-2OH C4H5OH-13 SQC4H7OHP-4 CY(CCCO)COH NC4KET21OH C2H5CHOHCO CH3COCOHCH3 C2H4COCH2OH CH3COHCO CH2COHCHO SQC4H7OHP-4O2 PQC4H7OHS-3O2 SQC4H7OHS-4O2 C4H7O2-1,3OOH NC4KET13OH-2 NC4KET24OH-1 NC4KET24OH-3 C4H6OHOOH1-4-3 C4H6OHOOH2-2-1 C4H6OHOOH1-3-4 C4H6OHOOH1-2-3 HOCH2CHO C4H71-4OOH C4H71-4O2 C4H61-3OOH4 C4H6O1-3OOH4 C4H6O2-1OOH4 HOCH2COCH2 HOCH2CO HOCHCHO PC3H4OH-3 PC3H4OH-1 CH3COCHOH SC2H2OH PC4H8OH-1 PC4H8OH-3 C4H7O1-4 PC4H8OH-4 SC4H8OH-2 CH2COHCO C4H72-2O2 C4H71-1O2 C4H71-2O2 C3H6OH1-1 PC4H8OH-2O2 SC4H8OH-1O2 C4H71-3OOCH3 C4H72-1OOCH3 C4H6 C4H612 C4H6-2 C4H5-I C4H5-N C4H5-2 C4H4 C4H3-I C4H3-N C4H2 C4H6O25 C2H3CHOCH2 C4H4O C4H6O23 CH2CHCHCHO H2C4O NC3H7CHO NC3H7CO C3H6CHO-1 C3H6CHO-2 C3H6CHO-3 SC3H5CHO SC3H5CO C2H5COCH3 C2H5COCH2 CH2CH2COCH3 CH3CHCOCH3 C2H3COCH3 CH3CHOOCOCH3 CH2CHOOHCOCH3 C2H5CHCO

NC5H12 C5H11-1 C5H11-2 C5H11-3 C5H11O2H-1 C5H11O2H-2 C5H11O2H-3 C5H11O2-1 C5H11O2-2 C5H11O2-3 C5H11O-1 C5H11O-2 C5H11O-3 C5H10OOH1-2 C5H10OOH1-3 C5H10OOH1-4 C5H10OOH1-5 C5H10OOH2-1 C5H10OOH2-3 C5H10OOH2-4 C5H10OOH2-5 C5H10OOH3-1 C5H10OOH3-2 C5H10O1-2 C5H10O1-3 C5H10O1-4 C5H10O1-5 C5H10O2-3 C5H10O2-4 C5H10OOH1-2O2 C5H10OOH1-3O2 C5H10OOH1-4O2 C5H10OOH1-5O2 C5H10OOH2-1O2 C5H10OOH2-3O2 C5H10OOH2-4O2 C5H10OOH2-5O2 C5H10OOH3-1O2 C5H10OOH3-2O2 C5H91-2,3OOH C5H91-2,4OOH C5H91-2,5OOH C5H91-3,4OOH C5H91-3,5OOH C5H91-4,5OOH C5H92-1,3OOH C5H92-1,4OOH C5H92-1,5OOH C5H92-3,4OOH C5H92-3,5OOH C5H92-4,5OOH C5H93-1,2OOH C5H93-1,4OOH C5H93-1,5OOH C5H93-2,4OOH C5H91-3OOH C5H91-4OOH C5H91-5OOH C5H92-1OOH C5H92-4OOH C5H92-5OOH C5H9O1-2OOH-3 C5H9O1-2OOH-4 C5H9O1-2OOH-5 C5H9O1-3OOH-2 C5H9O1-3OOH-4 C5H9O1-3OOH-5 C5H9O1-4OOH-2 C5H9O1-4OOH-3 C5H9O1-4OOH-5 C5H9O1-5OOH-2 C5H9O1-5OOH-3 C5H9O2-3OOH-1 C5H9O2-3OOH-4 C5H9O2-3OOH-5 C5H9O2-4OOH-1 C5H9O2-4OOH-3 C5H9O1-2O-5 CH2CH2OCH2CH2CHO NC5KET12 NC5KET13 NC5KET14 NC5KET15 NC5KET21 NC5KET23 NC5KET24 NC5KET25 NC5KET31 NC5KET32 NC5KET12O NC5KET13O NC5KET14O NC5KET15O NC5KET21O NC5KET23O NC5KET24O NC5KET25O NC5KET31O NC5KET32O NC5DIONE13 NC5DIONE24 C5H10OH23 O2C5H10OH23 OCH2CHO

CH2OCH2CHO C2H4OCHO C5H10OOH1-3OH C5H10OOH2-4OH C5H10OOH3-1OH NC5CYCPER13 NC5CYCPER24 NC5CYCPER31 IC5H12 AC5H11 BC5H11 CC5H11 DC5H11 AC5H9O-A2 AC5H11O2H BC5H11O2H CC5H11O2H DC5H11O2H AC5H11O2 BC5H11O2 CC5H11O2 DC5H11O2 AC5H11O BC5H11O CC5H11O DC5H11O AC5H10OOH-A AC5H10OOH-B AC5H10OOH-C AC5H10OOH-D BC5H10OOH-A BC5H10OOH-C BC5H10OOH-D CC5H10OOH-A CC5H10OOH-B CC5H10OOH-D DC5H10OOH-A DC5H10OOH-B DC5H10OOH-C A-AC5H10O A-BC5H10O A-CC5H10O A-DC5H10O B-CC5H10O B-DC5H10O C-DC5H10O AC5H10OOH-AO2 AC5H10OOH-BO2 AC5H10OOH-CO2 AC5H10OOH-DO2 BC5H10OOH-AO2 BC5H10OOH-CO2 BC5H10OOH-DO2 CC5H10OOH-AO2 CC5H10OOH-BO2 CC5H10OOH-DO2 DC5H10OOH-AO2 DC5H10OOH-BO2 DC5H10OOH-CO2 C5H9A-A,BOOH C5H9A-A,COOH C5H9A-A,DOOH C5H9A-B,COOH C5H9A-B,DOOH C5H9A-C,DOOH C5H9B-A,AOOH C5H9B-A,COOH C5H9B-A,DOOH C5H9B-C,DOOH C5H9C-A,AOOH C5H9C-A,BOOH C5H9C-A,DOOH C5H9C-B,DOOH C5H9D-A,AOOH C5H9D-A,BOOH C5H9D-A,COOH C5H9D-B,COOH C5H9A-AOOH C5H9A-COOH C5H9A-DOOH C5H9B-AOOH C5H9B-DOOH C5H9C-AOOH C5H9C-BOOH C5H9OA-AOOH-B C5H9OA-AOOH-C C5H9OA-AOOH-D C5H9OA-BOOH-A C5H9OA-BOOH-C C5H9OA-BOOH-D C5H9OA-COOH-A C5H9OA-COOH-B C5H9OA-COOH-D C5H9OA-DOOH-A C5H9OA-DOOH-B C5H9OA-DOOH-C C5H9OB-COOH-A C5H9OB-COOH-D C5H9OB-DOOH-A C5H9OB-DOOH-C C5H9OC-DOOH-A C5H9OC-DOOH-B CH3COCH2OCH2CH2 IC5KETAA IC5KETAB IC5KETAC IC5KETAD IC5KETCA IC5KETCB IC5KETCD IC5KETDA IC5KETDB IC5KETDC IC5KETAAO IC5KETABO IC5KETACO IC5KETADO IC5KETCAO IC5KETCBO IC5KETCDO IC5KETDAO IC5KETDBO IC5KETDCO AC5H10OH BC5H10OH CC5H10OH AO2C5H10OH BO2C5H10OH CO2C5H10OH IC3H5COCH3 IC3H5COCH2 AC3H4COCH3 NEOC5H12 NEOC5H11 NEOC5H11O2H NEOC5H11O2 NEOC5H11O NEOC5H10OOH NEO-C5H10O NEOC5H10OOH-O2 NEOC5H9Q2 NEOC5KET NEOC5KETOX NEOC5KEJOL IC4H6Q2-II NEOC5H9O-OOH C5H10-1 C5H10-2 C5H81-3 C5H91-3 C5H91-4 C5H91-5 C5H92-4 C5H92-5 C5H9O1-3 C5H9O2-4 BC5H10 CC5H10 CC5H9-A CC5H9-B AC5H9O-C CC5H9O-B AC5H10 AC5H9-A2 AC5H9-C AC5H9-D B2E2M1OJ B13DE2M B13DE2MJ B12DE3M B2E3M1OJ TC4H8CHO O2C4H8CHO O2HC4H8CO C5H8D14 C5H714-1 CVCCVCCJ PC4H8CHO-4 PC4H9CO C4H7CHO-4 PC4H9CHO PC4H8CHO-1O2 PC4H8CHO-2O2 PC4H8CHO-3O2 PC4H8CHO-4O2 C4H7CHO-2 C4H7CHO-3 PC4H8CHO-1 PC4H8CHO-2 PC4H8CHO-3 NC3H7COCH3 C2H5COC2H5 NC3H7COCH2 CH3CH2CHCOCH3 CH3CHCH2COCH3 CH2CH2CH2COCH3 CH2CH2COC2H5 CH3CHCOC2H5 NC52ONEO2-3 NC52ONEO2-4 NC52ONEO2-5 NC53ONEO2-1 NC53ONEO2-2 NC52ONE-3 NC52ONE-4 NC53ONE-1 NC5H11OH C5H10OH11 C5H10OH12 C5H10OH13 C5H10OH14 C5H10OH15 C5H10OH-1O2 C5H10OH-2O2 C5H10OH-3O2 C5H10OH-4O2 C5H10OH-5O2 C5H9OH1-1 C5H9OH1-2 C5H9OH1-3 C5H9OH1-4

NC6H14 C6H13-1 C6H13-2 C6H13-3 C6H13OOH-1 C6H13OOH-2 C6H13OOH-3 C6H13O2-1 C6H13O2-2 C6H13O2-3 C6H13O-1 C6H13O-2 C6H13O-3 C6H12OOH1-2 C6H12OOH1-3 C6H12OOH1-

4 C6H12OOH1-5 C6H12OOH2-1 C6H12OOH2-3 C6H12OOH2-4 C6H12OOH2-5 C6H12OOH2-6 C6H12OOH3-1 C6H12OOH3-2 C6H12OOH3-4 C6H12OOH3-5 C6H12OOH3-6 C6H12O1-2 C6H12O1-3 C6H12O1-4 C6H12O1-5 C6H12O2-3 C6H12O2-4 C6H12O2-5 C6H12O3-4 C6H12OOH1-2O2 C6H12OOH1-3O2 C6H12OOH1-4O2 C6H12OOH1-5O2 C6H12OOH2-1O2 C6H12OOH2-3O2 C6H12OOH2-4O2 C6H12OOH2-5O2 C6H12OOH2-6O2 C6H12OOH3-1O2 C6H12OOH3-2O2 C6H12OOH3-4O2 C6H12OOH3-5O2 C6H12OOH3-6O2 C6H11-1D3OOH C6H11-1D4OOH C6H11-1D5OOH C6H11-1D6OOH C6H11-2D1OOH C6H11-2D4OOH C6H11-2D5OOH C6H11-2D6OOH C6H11-3D1OOH C6H11-3D2OOH C6H11Q12-3 C6H11Q12-4 C6H11Q12-5 C6H11Q12-6 C6H11Q13-2 C6H11Q13-4 C6H11Q13-5 C6H11Q13-6 C6H11Q14-2 C6H11Q14-3 C6H11Q14-5 C6H11Q14-6 C6H11Q15-2 C6H11Q15-3 C6H11Q15-4 C6H11Q15-6 C6H11Q23-1 C6H11Q23-4 C6H11Q23-5 C6H11Q23-6 C6H11Q24-1 C6H11Q24-3 C6H11Q24-5 C6H11Q24-6 C6H11Q25-1 C6H11Q25-3 C6H11Q34-1 C6H11Q34-2 C6KET12 C6KET13 C6KET14 C6KET15 C6KET21 C6KET23 C6KET24 C6KET25 C6KET26 C6KET31 C6KET32 C6KET34 C6KET35 C6KET36 C5H91-1 C6H11O12-3OOH C6H11O12-4OOH C6H11O12-5OOH C6H11O12-6OOH C6H11O13-2OOH C6H11O13-4OOH C6H11O13-5OOH C6H11O13-6OOH C6H11O14-2OOH C6H11O14-3OOH C6H11O14-5OOH C6H11O14-6OOH C6H11O15-2OOH C6H11O15-3OOH C6H11O15-4OOH C6H11O15-6OOH C6H11O23-1OOH C6H11O23-4OOH C6H11O23-5OOH C6H11O23-6OOH C6H11O24-1OOH C6H11O24-3OOH C6H11O24-5OOH C6H11O24-6OOH C6H11O25-1OOH C6H11O25-3OOH C6H11O34-1OOH C6H11O34-2OOH C4H7O12-4 C4H7O13-4 C4H7O23-1 C5H9O12-5 C5H9O13-5 C5H9O14-5 C5H9O23-1 C5H9O23-5 C5H9O24-1 AC3H5CHO C6KET12O C6KET13O C6KET14O C6KET15O C6KET21O C6KET23O C6KET24O C6KET25O C6KET26O C6KET31O C6KET32O C6KET34O C6KET35O C6KET36O C6H12OOH1-2O C6H12OOH1-3O C6H12OOH1-4O C6H12OOH1-5O C6H12OOH2-1O C6H12OOH2-3O C6H12OOH2-4O C6H12OOH2-5O C6H12OOH2-6O C6H12OOH3-1O C6H12OOH3-2O C6H12OOH3-4O C6H12OOH3-5O C6H12OOH3-6O NC5H11CHO CH3COOH C2H5COOH C6H12-1 C6H12-2 C6H12-3 C6H111-3 C6H111-4 C6H111-5 C6H111-6 C6H112-4 C6H112-5 C6H112-6 C6H113-1 C6H12OH-1J2 C6H12OH-2J1 C6H12OH-2J3 C6H12OH-3J2 C6H12OH-3J4 C6H12OH-1O2-2 C6H12OH-2O2-1 C6H12OH-2O2-3 C6H12OH-3O2-2 C6H12OH-3O2-4 C6H11-1D3O C6H11-2D4O C6H10D14 C6H112O2-1 C6H111O2-3 C6H111O2-4 C6H111O2-5 C6H111O2-6 C6H112O2-4 C6H112O2-5 C6H112O2-6 C6H113O2-2 C6H113O2-1 C6H101OOH3-4 C6H101OOH3-5 C6H101OOH3-6 C6H101OOH4-3 C6H101OOH4-5 C6H101OOH4-6 C6H101OOH5-3 C6H101OOH5-4 C6H101OOH5-6 C6H101OOH6-3 C6H101OOH6-4 C6H101OOH6-5 C6H102OOH4-5 C6H102OOH4-6 C6H102OOH5-4 C6H102OOH5-6 C6H102OOH6-4 C6H102OOH6-5 C6H103OOH1-2 C6H103OOH2-1 ETES1 MVOX VTHF EDHF C6H101OOH3-4O2 C6H101OOH3-5O2 C6H101OOH3-6O2 C6H101OOH4-3O2 C6H101OOH4-5O2 C6H101OOH4-6O2 C6H101OOH5-3O2 C6H101OOH5-4O2 C6H101OOH5-6O2 C6H101OOH6-3O2 C6H101OOH6-4O2 C6H101OOH6-5O2 C6H102OOH4-5O2 C6H102OOH4-6O2 C6H102OOH5-4O2 C6H102OOH5-6O2 C6H102OOH6-4O2 C6H102OOH6-5O2 C6H103OOH1-2O2 C6H103OOH2-1O2 NC6D1KET34 NC6D1KET35 NC6D1KET36 NC6D1KET43 NC6D1KET45

NC6D1KET46 NC6D1KET53 NC6D1KET54 NC6D1KET56 NC6D1KET63 NC6D1KET64 NC6D1KET65 NC6D2KET45 NC6D2KET46 NC6D2KET54 NC6D2KET56 NC6D2KET64 NC6D2KET65 NC6D3KET12 NC6D3KET21 NC5H11CO NC5H10CHO-1 NC5H10CHO-2 NC5H10CHO-3 NC5H10CHO-4 NC5H10CHO-5 C6H10D13 C6H10D24 C6H101-5 C6H9-A C6H95-24 C6H96-24

IC6 IC6-1 IC6-2 IC6-3 IC6-4 IC6-5 IC6D1 IC6D2 IC6D3 IC6D4 IC6D1-1A IC6D1-3 IC6D1-4 IC6D1-5 IC6D2-5 IC6D3-1 IC6D3-2 IC6D4-1 IC6D4-2 IC6D4-3 IC6OH1-2J IC6OH2-1J IC6OH2-3J IC6OH3-2J IC6OH3-4J IC6OH4-3J IC6OH4-5J IC6OH5-4J IC6OH1-2O2 IC6OH2-1O2 IC6OH2-3O2 IC6OH3-2O2 IC6OH3-4O2 IC6OH4-3O2 IC6OH4-5O2 IC6OH5-4O2 IC6D1-3O IC6D3-2O IC6D4-3O IC6-1OOH IC6-2OOH IC6-3OOH IC6-4OOH IC6-5OOH IC6-1O2 IC6-2O2 IC6-3O2 IC6-4O2 IC6-5O2 IC6-1O IC6-2O IC6-3O IC6-4O IC6-5O IC6OOH1-1A IC6OOH1-2 IC6OOH1-3 IC6OOH1-4 IC6OOH1-5 IC6OOH2-1 IC6OOH2-3 IC6OOH2-4 IC6OOH2-5 IC6OOH3-1 IC6OOH3-2 IC6OOH3-4 IC6OOH3-5 IC6OOH4-1 IC6OOH4-2 IC6OOH4-3 IC6OOH4-5 IC6OOH5-1 IC6OOH5-2 IC6OOH5-3 IC6OOH5-4 IC6O1-1A IC6O1-2 IC6O1-3 IC6O1-4 IC6O1-5 IC6O2-3 IC6O2-4 IC6O2-5 IC6O3-4 IC6O3-5 IC6O4-5 IC6OOH1-1AO2 IC6OOH1-2O2 IC6OOH1-3O2 IC6OOH1-4O2 IC6OOH1-5O2 IC6OOH2-1O2 IC6OOH2-3O2 IC6OOH2-4O2 IC6OOH2-5O2 IC6OOH3-1O2 IC6OOH3-2O2 IC6OOH3-4O2 IC6OOH3-5O2 IC6OOH4-1O2 IC6OOH4-2O2 IC6OOH4-3O2 IC6OOH4-5O2 IC6OOH5-1O2 IC6OOH5-2O2 IC6OOH5-3O2 IC6OOH5-4O2 IC6Q11A-2 IC6Q12-1A IC6Q12-3 IC6Q13-2 IC6Q13-4 IC6Q14-2 IC6Q14-3 IC6Q14-5 IC6Q15-2 IC6Q15-4 IC6Q23-1 IC6Q23-4 IC6Q24-1 IC6Q24-3 IC6Q24-5 IC6Q25-1 IC6Q25-3 IC6Q25-4 IC6Q34-2 IC6Q34-5 IC6Q35-2 IC6Q35-4 IC6Q45-3 IC6KET1-1A IC6KET1-2 IC6KET1-3 IC6KET1-4 IC6KET1-5 IC6KET3-1 IC6KET3-2 IC6KET3-4 IC6KET3-5 IC6KET4-1 IC6KET4-2 IC6KET4-3 IC6KET4-5 IC6KET5-1 IC6KET5-2 IC6KET5-3 IC6KET5-4 IC6D1-1AOOH IC6D1-3OOH IC6D1-4OOH IC6D1-5OOH IC6D2-1OOH IC6D2-4OOH IC6D2-5OOH IC6D3-1OOH IC6D3-2OOH IC6D3-5OOH IC6D4-1OOH IC6D4-2OOH IC6D4-3OOH IC6O11A-2OOH IC6O12-1AOOH IC6O12-3OOH IC6O12-4OOH IC6O12-5OOH IC6O13-2OOH IC6O13-4OOH IC6O14-2OOH IC6O14-3OOH IC6O14-5OOH IC6O15-2OOH IC6O15-4OOH IC6O23-1OOH IC6O23-4OOH IC6O23-5OOH IC6O24-1OOH IC6O24-3OOH IC6O24-5OOH IC6O25-1OOH IC6O25-3OOH IC6O25-4OOH IC6O34-1OOH IC6O34-2OOH IC6O34-5OOH IC6O45-1OOH IC6O45-2OOH IC6O45-3OOH IC4H9CO IC6D13 SC4H9CHO IC6D1-1AO IC6Q11A-3 IC6Q11A-4 IC6Q11A-5 IC6Q12-4 IC6Q12-5 IC6Q13-1A IC6Q13-5 IC6Q14-1A IC6Q15-1A IC6Q15-3 IC6Q23-5 IC6Q34-1 IC6Q35-1 IC6Q45-1 IC6Q45-2 IC5Y3 IC6O35-2OOH IC6O35-4OOH C5H9O23-4 C5H9O12-4 IC3H7CHCO IC5O23-4J IC6O13-1AOOH IC6O14-1AOOH IC6O15-1AOOH IC6O11A-3OOH IC6O15-3OOH IC6O13-5OOH IC6O11A-4OOH IC6O11A-5OOH IC6O35-1OOH CC5H9-AO C5H9O2-5 CC4H7O-IJ A-AC5H10O-DJ A-BC5H10O-DJ C5H91-5O C5H91-4O C5H92-5O IC6KET1-1AO IC6KET1-2O IC6KET1-3O IC6KET1-4O IC6KET1-5O IC6KET3-1O IC6KET3-2O IC6KET3-4O IC6KET3-5O IC6KET4-1O IC6KET4-2O IC6KET4-3O IC6KET4-5O IC6KET5-1O IC6KET5-2O IC6KET5-3O IC6KET5-4O

I3C6 I3C6-1 I3C6-2 I3C6-3 I3C6-4 I3C6D1 I3C6D2 I3C6D3 I3C6D1-3 I3C6D1-4 I3C6D1-5 I3C6D1-6 I3C6D2-5 I3C6D2-6 I3C6D3-1 I3C6D3-2 I3C6OH1-2J I3C6OH2-1J I3C6OH2-3J I3C6OH3-2J I3C6OH3-4J I3C6OH4-3J I3C6OH1-2O2 I3C6OH2-1O2 I3C6OH2-3O2 I3C6OH3-2O2 I3C6OH3-4O2 I3C6OH4-3O2 I3C6D1-3O I3C6D1-4O I3C6D1-5O I3C6D1-6O I3C6D2-5O I3C6D2-6O I3C6D3-1O I3C6D3-2O I3C6-1OOH I3C6-1O2 I3C6-2OOH I3C6-2O2 I3C6-3OOH I3C6-3O2 I3C6-4OOH I3C6-4O2 I3C6-1O I3C6-2O I3C6-3O I3C6-4O I3C6OOH1-2 I3C6OOH1-3 I3C6OOH1-4 I3C6OOH1-5 I3C6OOH1-6 I3C6OOH2-1 I3C6OOH2-3 I3C6OOH2-4 I3C6OOH2-5 I3C6OOH2-6 I3C6OOH3-1 I3C6OOH3-2 I3C6OOH3-4 I3C6OOH4-1 I3C6OOH4-2 I3C6OOH4-3 I3C6O1-2 I3C6O1-3 I3C6O1-4 I3C6O1-5 I3C6O1-6 I3C6O2-3 I3C6O2-4 I3C6O2-5 I3C6O3-4 I3C6OOH1-2O2 I3C6OOH1-3O2 I3C6OOH1-4O2 I3C6OOH1-5O2 I3C6OOH1-6O2 I3C6OOH2-1O2 I3C6OOH2-3O2 I3C6OOH2-4O2 I3C6OOH2-5O2 I3C6OOH2-6O2 I3C6OOH3-1O2 I3C6OOH3-2O2 I3C6OOH3-4O2 I3C6OOH4-1O2 I3C6OOH4-2O2 I3C6OOH4-3O2 I3C6KET1-2 I3C6KET1-3 I3C6KET1-4 I3C6KET1-5 I3C6KET1-6 I3C6KET2-1 I3C6KET2-3 I3C6KET2-4 I3C6KET2-5 I3C6KET2-6 I3C6KET4-1 I3C6KET4-2 I3C6KET4-3 I3C6D1-3OOH I3C6D1-4OOH I3C6D1-5OOH I3C6D1-6OOH I3C6D2-1OOH I3C6D2-4OOH I3C6D2-5OOH I3C6D2-6OOH I3C6D3-1OOH I3C6D3-2OOH I3C6Q12-3 I3C6Q12-4 I3C6Q12-5 I3C6Q12-6 I3C6Q13-2 I3C6Q13-4 I3C6Q13-5 I3C6Q13-6 I3C6Q14-2 I3C6Q14-3 I3C6Q14-5 I3C6Q14-6 I3C6Q15-2 I3C6Q15-3 I3C6Q15-4 I3C6Q15-6 I3C6Q16-2 I3C6Q16-3 I3C6Q16-4 I3C6Q23-1 I3C6Q23-4 I3C6Q23-5 I3C6Q23-6 I3C6Q24-1 I3C6Q24-3 I3C6Q24-5 I3C6Q24-6 I3C6Q25-1 I3C6Q25-3 I3C6Q25-4 I3C6Q34-1 I3C6Q34-2 I3C6O12-3OOH I3C6O12-4OOH I3C6O12-5OOH I3C6O12-6OOH I3C6O13-2OOH I3C6O13-4OOH I3C6O13-5OOH I3C6O13-6OOH I3C6O14-2OOH I3C6O14-3OOH I3C6O14-5OOH I3C6O14-6OOH I3C6O15-2OOH I3C6O15-3OOH I3C6O15-4OOH I3C6O15-6OOH I3C6O16-2OOH I3C6O16-3OOH I3C6O16-4OOH I3C6O23-1OOH I3C6O23-4OOH I3C6O23-5OOH I3C6O23-6OOH I3C6O24-1OOH I3C6O24-3OOH I3C6O24-5OOH I3C6O24-6OOH I3C6O25-1OOH I3C6O25-3OOH I3C6O25-4OOH I3C6O34-1OOH I3C6O34-2OOH IC5Y3-1J C5H9O2-1 IC5O34-1J C5H9O15-3 AC5H9O-D SC4H9CO SC4H8CHO-1 SC4H8CHO-2 SC4H8CHO-3 I3C6KET1-2O I3C6KET1-3O I3C6KET1-4O I3C6KET1-5O I3C6KET1-6O I3C6KET2-1O I3C6KET2-3O I3C6KET2-4O I3C6KET2-5O I3C6KET2-6O I3C6KET4-1O I3C6KET4-2O I3C6KET4-3O

NEC6 NEC6-1 NEC6-3 NEC6-4 NEC6D3 NEC6D3-1 NEC6OH3-4J NEC6OH4-3J NEC6OH3-4O2 NEC6OH4-3O2 NEC6-1OOH NEC6-1O2 NEC6-3OOH NEC6-3O2 NEC6-4OOH NEC6-4O2 NEC6-1O NEC6-3O NEC6-4O NEC6OOH1-1A NEC6OOH1-3 NEC6OOH1-4 NEC6OOH3-1 NEC6OOH3-4 NEC6OOH4-1 NEC6OOH4-3 NEC6O1-1A NEC6O1-3 NEC6O1-4 NEC6O3-4 NEC6OOH1-1AO2 NEC6OOH1-3O2 NEC6OOH1-4O2 NEC6OOH3-1O2 NEC6OOH3-4O2 NEC6OOH4-1O2 NEC6OOH4-3O2 NEC6KET1-1A NEC6KET1-3 NEC6KET1-4 NEC6KET3-1 NEC6KET3-4 NEC6KET4-1 NEC6KET4-3 NEC6D3-1OOH NEC6Q11A-1B NEC6Q11A-3 NEC6Q11A-4 NEC6Q13-1A NEC6Q13-4 NEC6Q14-1A NEC6Q14-3 NEC6Q34-1 NEC6KET1-1AO NEC6KET1-3O NEC6KET1-4O NEC6KET3-1O NEC6KET3-

4O NEC6KET4-1O NEC6KET4-3O NEC6O11A-1BOOH NEC6O11A-3OOH NEC6O11A-4OOH NEC6O13-1AOOH NEC6O13-4OOH NEC6O14-1AOOH NEC6O14-3OOH NEC6O34-1OOH TC4H9CHO TC4H9CO IC5Y3-2J

XC6 XC6-1 XC6-2 XC6D1 XC6D2 XC6D1-1A XC6D1-3 XC6OH1-2J XC6OH2-1J XC6OH2-3J XC6OH1-2O2 XC6OH2-1O2 XC6OH2-3O2 XC6-1OOH XC6-1O2 XC6-2OOH XC6-2O2 XC6-1O XC6-2O XC6OOH1-1A XC6OOH1-2 XC6OOH1-3 XC6OOH1-4 XC6OOH2-1 XC6OOH2-3 XC6OOH2-4 XC6O1-1A XC6O1-2 XC6O1-3 XC6O1-4 XC6O2-3 XC6OOH1-1AO2 XC6OOH1-2O2 XC6OOH1-3O2 XC6OOH1-4O2 XC6OOH2-1O2 XC6OOH2-3O2 XC6OOH2-4O2 XC6KET1-1A XC6KET1-2 XC6KET1-3 XC6KET1-4 XC6D1-1AOOH XC6D2-1OOH XC6D1-4OOH XC6D1-3OOH XC6Q11A-2 XC6Q11A-3 XC6Q11A-4 XC6Q12-1A XC6Q12-3 XC6Q12-4 XC6Q13-1A XC6Q13-2 XC6Q13-4 XC6Q14-1A XC6Q14-2 XC6Q23-1 XC6KET1-1AO XC6KET1-2O XC6KET1-3O XC6KET1-4O XC6O11A-2OOH XC6O11A-3OOH XC6O11A-4OOH XC6O12-1AOOH XC6O12-3OOH XC6O12-4OOH XC6O13-1AOOH XC6O13-2OOH XC6O13-4OOH XC6O14-1AOOH XC6O14-2OOH XC6O23-1OOH C4H72-2CHO XC6D1-4 XC6D1-1AO XC6D1-3O BC5H9O-A CC5H9O-A

H15DE25DM H15DE25DM-S H15DE25DM-A H15DE25DM-AO H15DE25DM-SO H15DE2M-T IC4H7CHO C3Y12 C3Y12-1R DC5H10O DC5H9O-C IC6D13-1AR DC5H9O-B IC5D2Y4 IC6D13-5R IC6D24 NC5D124 NC5D124-5R DC5H9O-A C4H8CHO4-2 IC3H7COCH2 NC6D14 IC6D14 IC6D14-1 I3C6D13 I3C6D15 I3C6D25 I3C6D13-5 I3C6D13-6 I3C6D15-3 I3C6D15-4 XC6D13 XC6D13-1AR C6Y2-1J NC5CO3 PC4H9CO3 NC3H7CO3 C2H5CO3 NC5CO3H PC4H9CO3H NC3H7CO3H C2H5CO3H C2H5COC2H3 PC2H4COC2H3 SC2H4COC2H3 C6H9-AOOH TC4H9CO3 IC3H7CO3 TC4H9CO3H IC3H7CO3H C4D13KET C5H3O-3 C5H4O C5H4OH C5H5 C5H5CH3 C5H5CH3-1 C5H5CH3-2 C5H5O C5H5OH C5H5OO C5H5OOH C5H6 C6H2 C6H3 C6H4OH C6H5 C6H5O C6H5OH C6H5OO C6H5OOH C6H6 C6H6O-24 C6H6O-25 C6H6O-B1 C-C6H4 CJVCCVCCVO CJVCCVCVO CJVCCVO CVCCVCCJVO CVCCVCCVO CYC5H71-3 CYC5H71-4 FULVENE HOC6H4CH3 L-C6H4 O-C6H4O2 O-HOC6H4OH O-OC6H4OH O-OOC6H4OH OVCCVCCJVO OVCCVCCVO OVCCVCVO P-C6H3O2 P-C6H4O2 P-HOC6H4OH P-OC6H4OH P-OOC6H4OH C6H5CH2 C6H5CH3

CPT CYC5H9 CYC5H8 CYC5H71-4 CYC5H71-3 CYC51EN3OJ CPTO2J CPT1Q2J CPT1Q3J PT1N3Q5J PT1N1Q5J PT1N4Q5J CPTYO12 CPTYO13 CPTO CPTO2H CPTOJ CPTQ2QJ CPTQ3QJ CPT1*O2Q CPT1*O3Q PT1N3*O5J CPTYO123J CYC5O1EN5J C53OH1EN5J C4H6CHO2-5 C4H6CHO4-5 C2H3OC3H4A C4H7CO1-4 C4H6CHO1-43

MCP MCPR1 MCPR2 MCPR3 CPTCH2 MCYC5-1N MCYC5-2N MCYC5-3N MCYC5-4N MCYC51N3J MCYC51N4J MCYC52N6J MCYC52N4J MCYC52N5J MCYC53N1J MCYC53N5J MCYC53N6J MCYC54N1J MCYC54N2J MCYC5-13N MCYC5-14N MCYC5-25N MCYC5-24N MCYC5-35N MCYC513N6 MCYC513N5 MCYC525N4 MCYC535N1 MCYC54N3J MCPR1O2J MCPR2O2J MCPR3O2J CPTCH2O2J

MCPR1OJ MCPR2OJ MCPR3OJ CPTCH2OJ MCPR1QMJ MCPR1Q2J MCPR1Q3J MCPR2QMJ MCPR2Q1J MCPR2Q3J MCPR2Q4J MCPR2Q5J MCPR3Q2J MCPR3Q1J MCPR3QMJ MCPR3Q4J MCPR3Q5J CPTCH2Q1J CPTCH2Q2J CPTCH2Q3J MCPR1O2H MCPR2O2H MCPR3O2H CPTCH2O2H MCPYO1CH2 MCPYO12 MCPYO13 MCPYO2CH2 MCPYO23 MCPYO24 MCPYO25 MCPYO3CH2 MCPYO34 MCPR1QMQJ MCPR1Q2QJ MCPR1Q3QJ MCPR2QMQJ MCPR2Q1QJ MCPR2Q3QJ MCPR2Q4QJ MCPR2Q5QJ MCPR3Q2QJ MCPR3Q1QJ MCPR3QMQJ MCPR3Q4QJ MCPR3Q5QJ CPTCH2Q1Q CPTCH2Q2Q CPTCH2Q3Q MCP2*OMQ MCP2*O1Q MCP2*O3Q MCP2*O4Q MCP2*O5Q MCP3*O2Q MCP3*O1Q MCP3*OMQ MCP3*O4Q MCP3*O5Q CPTCH2*O1 CPTCH2*O2 CPTCH2*O3 MCP1QMQ2J MCP1NMQ MCP1Q2Q5J MCP1N5Q MCP1Q2QMJ MCP1Q2Q4J MCPMN2Q MCPR1Q3QJ MCP1Q3Q5J MCP1N4Q MCPM*O1J MCP2*O1J MCP3*O1J MCP2*OMJ MCPM*O2J MCP3*O2J MCP2*O3J MCP2*O4J MCP3*O5J MCP2*O5J MCP3*OMJ MCPM*O3J MCP3*O4J CPT1*O2J CPT1*O3J CPT1N1Q CPT1*O2*O CPT1*O3*O CPT1O2O3J CPT1O3O2J CPT1O3O4J mcp2d mcp2dp mcp2dt C4H8COCH3-1 C5H10CHO5-2 AC5H10CHO C4CHO3M1J C62*O5N C5H9CHO1N C5H9CHO-2 C5H9CHO2N C5H9CHO-4 C5H9CHO-3 C5CHO2N2Q C4CHO1N4M4Q C61N4Q5*O C5CHO1N2Q C4CHO1N3M3Q C5H9CO1N C5H9CO2N C5H9CO-4 C5H9CO-3 C5H9CO-2 C62*O5N1J MCYC51N3OJ C6H9O-1 MCYC52N4OJ C6H9O-2 CH3CCHCHO MCYC52N6OJ C6H9O-3 CHC(CH3)CHO CH2C(CH2)CHO MCYC53N5OJ C6H9O-4

END REACTIONS H2+M=H+H+M 4.580E+19 -1.400 104400.0 H2 / 2.500 / H2O / 12.000 / CO / 1.900 / CO2 / 3.800 / HE / 0.830 / CH4 / 2.000 / C2H6 / 3.000 / CH3+H(+M)=CH4(+M) 1.270E+16 -0.630 383.0 LOW / 2.480E+33 -4.760 2440.0 / TROE / 7.830E-01 7.400E+01 2.941E+03 6.964E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ CH4+H=CH3+H2 6.140E+05 2.500 9587.0 CH4+O=CH3+OH 1.020E+09 1.500 8600.0 CH4+OH=CH3+H2O 5.830E+04 2.600 2190.0 CH4+HO2=CH3+H2O2 1.410E+01 3.740 21010.0 CH4+CH3O2=CH3+CH3O2H 9.600E-01 3.770 17810.0 CH3+HO2=CH4+O2 1.160E+05 2.230 -3022.0 CH4+CH2=CH3+CH3 2.460E+06 2.000 8270.0 CH2(S)+N2=CH2+N2 1.500E+13 0.000 600.0 CH2(S)+AR=CH2+AR 9.000E+12 0.000 600.0 CH2(S)+H2O=CH2+H2O 3.000E+13 0.000 0.0

CH2+H(+M)=CH3(+M) 2.500E+16 -0.800 0.0 LOW / 3.200E+27 -3.140 1230.0 / TROE / 6.800E-01 7.800E+01 1.995E+03 5.590E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/

CHV+AR=CH+AR 4.000E+11 0.500 0.0 CHV+H2O=CH+H2O 5.300E+13 0.000 0.0 CHV+CO=CH+CO 2.440E+12 0.500 0.0 CHV+CO2=CH+CO2 2.410E-01 4.300 -1694.0 CHV+O2=CH+O2 2.480E+06 2.140 -1720.0 CHV+H2=CH+H2 1.470E+14 0.000 1361.0 CHV+CH4=CH+CH4 1.730E+13 0.000 167.0 CHV=CH 1.860E+06 0.000 0.0 CHV+N2=CH+N2 3.030E+02 3.400 -381.0 C+H+M=CHV+M

6.000E+14 0.000 6940.0 CH+O2=CO+OHV 4.040E+13 0.000 0.0 CH+O2=HCO+O 3.300E+13 0.000 0.0

CH+H=C+H2 1.100E+14 0.000 0.0 CH+OH=HCO+H 3.000E+13 0.000 0.0

CH3O+CH3O=CH3OH+CH2O 6.030E+13 0.000 0.0 HCOH+O2=¿CO2+H+OH 5.000E+12 0.000 0.0 HCOH+O2=CO2+H2O 3.000E+13 0.000 0.0 HCOH+O=¿CO2+H+H 5.000E+13 0.000 0.0 HCOH+O=¿CO+OH+H 3.000E+13 0.000 0.0 HCOH+H=CH2O+H 2.000E+14 0.000 0.0 HCOH+OH=HCO+H2O 2.000E+13 0.000 0.0 HCO+H(+M)=CH2O(+M) 1.090E+12 0.480 -260.0 LOW / 1.350E+24 -2.570 1425.0 / TROE / 7.824E-01 2.710E+02 2.755E+03 6.570E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ CO+H2(+M)=CH2O(+M) 4.300E+07 1.500 79600.0 LOW / 5.070E+27 -3.420 84348.0 / TROE / 9.320E-01 1.970E+02 1.540E+03 1.030E+04 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ CH2O+O2=HCO+HO2 8.070E+15 0.000 53420.0 CH2O+O=HCO+OH 6.260E+09 1.150 2260.0 CH2O+H=HCO+H2 5.740E+07 1.900 2740.0 CH2O+OH=HCO+H2O 7.820E+07 1.630 -1055.0 CH2O+HO2=HCO+H2O2 1.880E+04 2.700 11520.0 CH2O+CH3=HCO+CH4 3.830E+01 3.360 4312.0 CH2O+O2CHO=HCO+HO2CHO 1.990E+12 0.000 11660.0 CH2O+OCHO=HCO+HOCHO 5.600E+12 0.000 13600.0 CH2O+CH3O=HCO+CH3OH 6.620E+11 0.000 2294.0 CH2O+CH3O2=HCO+CH3O2H 1.990E+12 0.000 11660.0 HCO+M=H+CO+M 5.700E+11 0.660 14870.0 H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HCO+O2=CO+HO2 7.580E+12 0.000 410.0 HCO+O=CO+OH 3.020E+13 0.000 0.0 HCO+H=CO+H2 7.340E+13 0.000 0.0 HCO+OH=CO+H2O 3.010E+13 0.000 0.0 HCO+CH3=CH4+CO 2.650E+13 0.000 0.0 HCO+HCO=CH2O+CO 1.800E+13 0.000 0.0 HCO+O=CO2+H 3.000E+13 0.000 0.0 HCO+HO2=¿CO2+H+OH 3.000E+13 0.000 0.0 HCO+HCO=¿H2+CO+CO 3.000E+12 0.000 0.0 CH2O+H(+M)=CH2OH(+M) 5.400E+11 0.454 3600.0 LOW / 1.270E+32 -4.820 6530.0 / TROE / 7.187E-01 1.030E+02 1.291E+03 4.160E+03 / H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ CH3O(+M)=CH2O+H(+M) 6.800E+13 0.000 26170.0 LOW / 1.870E+25 -3.000 24307.0 / TROE / 9.000E-01 2.500E+03 1.300E+03 1.000E+99 / H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ CH2O+OH=HOCH2O 4.500E+15 -1.100 0.0 HOCH2O=HOCHO+H 1.000E+14 0.000 14900.0 CH2O+HO2=OCH2O2H 1.500E+11 0.000 11900.0 OCH2O2H=HOCH2O2 3.000E+11 0.000 8600.0 HOCH2O2+HO2=HOCH2O2H+O2 3.500E+10 0.000 -3275.0 HOCH2O+OH=HOCH2O2H 1.000E+13 0.000 0.0 HCO+O2=O2CHO 1.200E+11 0.000 -1100.0 HOCHO=CO+H2O 2.450E+12 0.000 60470.0 HOCHO=CO2+H2 2.950E+09 0.000 48520.0 OCHO+HO2=HOCHO+O2 3.500E+10 0.000 -3275.0 OCHO+H2O2=HOCHO+HO2 2.400E+12 0.000 10000.0 HOCHO+H=¿H2+CO2+H 4.240E+06 2.100 4868.0 HOCHO+H=¿H2+CO+OH 6.030E+13 -0.350 2988.0 HOCHO+O=¿CO+OH+OH 1.770E+18 -1.900 2975.0 HOCHO+OH=¿H2O+CO2+H 2.620E+06 2.060 916.0 HOCHO+OH=¿H2O+CO+OH 1.850E+07 1.510 -962.0 HOCHO+CH3=¿CH4+CO+OH

3.900E-07 5.800 2200.0 HOCHO+HO2=¿H2O2+CO+OH 1.000E+12 0.000 11920.0 OCHO+OH=HO2CHO 2.000E+13 0.000 0.0 CH3+CH3(+M)=C2H6(+M) 2.280E+15 -0.690 175.0 LOW / 8.050E+31 -3.750 982.0 / TROE / 0.000E+00 5.700E+02 1.000E+30 1.000E+30 / H2O/ 5.00/ CO/ 2.00/ CO2/ 3.00/ C2H5+H(+M)=C2H6(+M) 5.210E+17 -0.990 1580.0 LOW / 1.990E+41 -7.080 6685.0 / TROE / 8.420E-01 1.250E+02 2.219E+03 6.882E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ C2H6+O2=C2H5+HO2 6.030E+13 0.000 51870.0 C2H6+O=C2H5+OH 3.550E+06 2.400 5830.0 C2H6+H=C2H5+H2 1.150E+08 1.900 7530.0 C2H6+OH=C2H5+H2O 1.480E+07 1.900 950.0 C2H6+HO2=C2H5+H2O2 3.460E+01 3.610 16920.0 C2H6+CH=C2H5+CH2 1.100E+14 0.000 -260.0 C2H6+CH2(S)=C2H5+CH3 1.200E+14 0.000 0.0 C2H6+CH3=C2H5+CH4 5.550E-04 4.720 3231.0 C2H6+CH3O=C2H5+CH3OH 2.410E+11 0.000 7090.0 C2H6+CH3O2=C2H5+CH3O2H 1.940E+01 3.640 17100.0 C2H6+C2H5O2=C2H5+C2H5O2H 8.600E+00 3.760 17200.0 C2H4+H(+M)=C2H5(+M) 9.570E+08 1.463 1355.0 LOW / 1.420E+39 -6.642 5769.0 / TROE / -5.690E-01 2.990E+02 -9.147E+03 1.524E+02 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ C2H5+H=C2H4+H2 2.000E+12 0.000 0.0 C2H4+C2H4=C2H5+C2H3 4.820E+14 0.000 71530.0 C2H5+CH3=CH4+C2H4 1.180E+04 2.450 -2921.0 C2H5+O=CH3CHO+H 1.100E+14 0.000 0.0 C2H5+HO2=C2H5O+OH 1.100E+13 0.000 0.0 C2H5+CH3O2=C2H5O+CH3O 8.000E+12 0.000 -1000.0 CH3+CH3=H+C2H5 4.740E+12 0.105 10664.0 PLOG / 1.00E-02 4.740E+12 0.105 10664.0 / PLOG / 1.00E-01 2.570E+13 -0.096 11406.0 / PLOG / 1.00E+00 3.100E+14 -0.362 13372.0 / PLOG / 1.00E+01 2.150E+10 0.885 13532.0 / PLOG / 1.00E+02 1.030E+02 3.230 11236.0 / C2H5+O2=C2H5O2 3.400E+53 -13.900 9279.0 PLOG / 4.00E-02 3.400E+53 -13.900 9279.0 / PLOG / 1.00E+00 9.360E+59 -15.280 14240.0 / PLOG / 1.00E+01 1.260E+60 -14.910 16240.0 /

C2H5+O2=C2H4O2H 2.100E+34 -9.010 5444.0 PLOG / 4.00E-02 2.100E+34 -9.010 5444.0 / PLOG / 1.00E+00 4.880E+33 -8.310 7710.0 / PLOG / 1.00E+01 1.710E+45 -11.490 14590.0 /

C2H5+O2=C2H4+HO2 2.090E+09 0.490 -391.0 PLOG / 4.00E-02 2.090E+09 0.490 -391.0 / PLOG / 1.00E+00 1.840E+07 1.130 -721.0 / PLOG / 1.00E+01 7.560E+14 -1.010 4749.0 /

C2H5+O2=C2H4O1-2+OH 1.300E+03 1.930 -503.0 PLOG / 4.00E-02 1.300E+03 1.930 -503.0 / PLOG / 1.00E+00 2.440E+02 2.180 -62.0 / PLOG / 1.00E+01 4.620E+09 0.150 5409.0 /

C2H5+O2=CH3CHO+OH 4.910E-06 4.760 254.0 PLOG / 4.00E-02 4.910E-06 4.760 254.0 / PLOG / 1.00E+00 6.800E-02 3.570 2643.0 / PLOG / 1.00E+01 8.260E+02 2.410 5285.0 /

C2H4O2H=C2H5O2 2.650E-16 6.960 2396.0 PLOG / 4.00E-02 2.650E-16 6.960 2396.0 / PLOG / 1.00E+00 1.060E+41 -10.100 26030.0 / PLOG / 1.00E+01 1.200E+36 -8.130 27020.0 /

C2H5O2=CH3CHO+OH 1.240E+35 -9.420 36360.0 PLOG / 4.00E-02 1.240E+35 -9.420 36360.0

/ PLOG / 1.00E+00 1.690E+36 -9.220 38700.0 / PLOG / 1.00E+01 2.520E+41 -10.200 43710.0 /

C2H5O2=C2H4+HO2 1.780E+32 -7.100 32840.0 PLOG / 4.00E-02 1.780E+32 -7.100 32840.0 / PLOG / 1.00E+00 2.700E+37 -8.470 35840.0 / PLOG / 1.00E+01 1.980E+38 -8.460 37900.0 /

C2H5O2=C2H4O1-2+OH 5.780E+45 -11.900 4112.0 PLOG / 4.00E-02 5.780E+45 -11.900 4112.0 / PLOG / 1.00E+00 1.920E+43 -10.750 42400.0 / PLOG / 1.00E+01 3.960E+43 -10.460 45580.0 /

C2H4O2H=C2H4O1-2+OH 8.960E+38 -9.400 20660.0 PLOG / 4.00E-02 8.960E+38 -9.400 20660.0 / PLOG / 1.00E+00 1.220E+37 -8.320 21460.0 / PLOG / 1.00E+01 8.850E+30 -6.080 20660.0 /

C2H4O2H=C2H4+HO2 3.920E+40 -10.200 22250.0 PLOG / 4.00E-02 3.920E+40 -10.200 22250.0 / PLOG / 1.00E+00 6.820E+40 -9.610 23840.0 / PLOG / 1.00E+01 3.980E+34 -7.250 23250.0 /

C2H4O2H=CH3CHO+OH 5.820E+26 -7.970 20860.0 PLOG / 4.00E-02 5.820E+26 -7.970 20860.0 / PLOG / 1.00E+00 5.520E+34 -9.880 26230.0 / PLOG / 1.00E+01 1.190E+34 -9.020 29210.0 / H2+C2H5O2=H+C2H5O2H 1.500E+14 0.000 26030.0 C2H5O2+HO2=C2H5O2H+O2 1.750E+10 0.000 -3275.0 C2H5O2+CH2O=C2H5O2H+HCO 1.990E+12 0.000 11660.0 C2H5O2+CH4=C2H5O2H+ 1.810E+11 0.000 18480.0 C2H5O2+CH3OH=C2H5O2H+CH2OH 1.810E+12 0.000 13710.0 C2H5O2H=C2H5O+O 6.310E+14 0.000 42300.0 C2H4O1-2=CH3+HCO 3.630E+13 0.000 57200.0 C2H4O1-2=CH3CHO 7.410E+12 0.000 53800.0 C2H4O1-2+H=C2H3O1-2+H2 8.000E+13 0.000 9680.0 C2H4O1-2+OH=C2H3O1-2+H2O 1.780E+13 0.000 3610.0 C2H4O1-2+HO2=C2H3O1-2+H2O2 1.130E+13 0.000 30430.0 C2H4O1-2+CH3=C2H3O1-2+CH4 1.070E+12 0.000 11830.0 C2H4O1-2+CH3O=C2H3O1-2+CH3OH 1.200E+11 0.000 6750.0 C2H4O1-2+CH3O2=C2H3O1-2+CH3O2H 1.130E+13 0.000 30430.0 C2H4O1-2+C2H5O2=C2H3O1-2+C2H5O2H 1.130E+13 0.000 30430.0 C2H3O1-2=CH3CO 8.500E+14 0.000 14000.0 C2H3O1-2=CH2CHO 1.000E+14 0.000 14000.0 C2H3+H(+M)=C2H4(+M) 6.080E+12 0.270 280.0 LOW / 1.400E+30 -3.860 3320.0 / TROE / 7.820E-01 2.075E+02 2.663E+03 6.095E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ C2H4(+M)=H2+H2CC(+M) 8.000E+12 0.440 88770.0 LOW / 7.000E+50 -9.310 99860.0 / TROE / 7.345E-01 1.800E+02 1.035E+03 5.417E+03 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ C2H4+O2=C2H3+HO2 4.220E+13 0.000 57623.0 C2H4+H=C2H3+H2 5.070E+07 1.930 12950.0 C2H4+OH=C2H3+H2O 2.230E+04 2.745 2216.0 C2H4+CH3O=C2H3+CH3OH 1.200E+11 0.000 6750.0 C2H4+CH3O2=C2H3+CH3O2H 8.590E+00 3.754 27132.0 C2H4+C2H5O2=C2H3+C2H5O2H 8.590E+00 3.754 27132.0 C2H4+CH3CO3=C2H3+CH3CO3H

1.130E+13 0.000 30430.0 C2H4+CH3=C2H3+CH4 9.760E+02 2.947 15148.0 DUP C2H4+CH3=C2H3+CH4 8.130E-05 4.417 8836.0 DUP C2H4+O=CH3+HCO 7.450E+06 1.880 183.0 C2H4+O=CH2CHO+H 6.100E+06 1.880 183.0 CH+CH4=C2H4+H 6.000E+13 0.000 0.0 CH2(S)+CH3=C2H4+H 2.000E+13 0.000 0.0 C2H4+OH=CH3+CH2O 5.350E+00 2.920 -1733.0 PLOG / 1.00E-02 5.350E+00 2.920 -1733.0 / PLOG / 2.50E-02 3.190E+01 2.710 -1172.0 / PLOG / 1.00E-01 5.550E+02 2.360 -181.0 / PLOG / 1.00E+00 1.780E+05 1.680 2060.0 / PLOG / 1.00E+01 2.370E+09 0.560 6007.0 / PLOG / 1.00E+02 2.760E+13 -0.500 11455.0 / C2H4+OH=CH3CHO+H 2.370E-07 5.300 -2051.0 PLOG / 1.00E-02 2.370E-07 5.300 -2051.0 / PLOG / 2.50E-02 8.730E-05 4.570 -618.0 / PLOG / 1.00E-01 4.030E-01 3.540 1882.0 / PLOG / 1.00E+00 2.380E-02 3.910 1723.0 / PLOG / 1.00E+01 8.250E+08 1.010 10507.0 / PLOG / 1.00E+02 6.800E+09 0.810 13867.0 / C2H4+OH=C2H3OH+H 1.040E+04 2.600 4121.0 PLOG / 1.00E-02 1.040E+04 2.600 4121.0 / PLOG / 2.50E-02 1.070E+04 2.600 4129.0 / PLOG / 1.00E-01 1.520E+04 2.560 4238.0 / PLOG / 1.00E+00 3.190E+05 2.190 5256.0 / PLOG / 1.00E+01 1.940E+08 1.430 7829.0 / PLOG / 1.00E+02 8.550E+10 0.750 11491.0 / C2H4+OH=PC2H4OH 1.740E+43 -10.461 7699.0 PLOG / 1.00E-02 1.740E+43 -10.461 7699.0 / PLOG / 2.50E-02 3.250E+37 -8.629 5215.0 / PLOG / 1.00E-01 1.840E+35 -7.750 4909.0 / PLOG / 1.00E+00 2.560E+36 -7.752 6946.0 / PLOG / 1.00E+01 3.700E+33 -6.573 7606.0 / PLOG / 1.00E+02 1.120E+26 -4.101 5757.0 / C2H4+HO2=C2H4O1-2+OH 3.340E+12 0.000 17190.0 C2H4+CH3O2=C2H4O1-2+CH3O 2.820E+12 0.000 17110.0 C2H4+C2H5O2=C2H4O1-2+C2H5O 2.820E+12 0.000 17110.0 C2H2+H(+M)=C2H3(+M) 1.710E+10 1.266 2709.0 LOW / 6.350E+31 -4.664 3780.0 / TROE / 7.880E-01 -1.020E+04 1.000E-30 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ C2H3+O2=C2H3OO 4.070E+27 -4.670 5222.0 PLOG / 1.00E-02 1.550E+24 -5.450 9662.0 / PLOG / 1.00E-01 3.480E+56 -15.010 19160.0 / PLOG / 3.16E-01 1.250E+64 -16.970 21290.0 / PLOG / 1.00E+00 3.340E+61 -15.790 20150.0 / PLOG / 3.16E+00 7.340E+53 -13.110 17300.0 / PLOG / 1.00E+01 4.160E+48 -11.210 16000.0 / PLOG / 3.16E+01 2.330E+43 -9.380 14810.0 / PLOG / 1.00E+02 3.410E+39 -8.040 14360.0 / DUP C2H3+O2=C2H3OO 4.070E+27 -4.670 5222.0 PLOG / 1.00E-02 1.780E-09 4.150 -4707.0 / PLOG / 1.00E-01 2.360E+22 -4.520 2839.0 / PLOG / 3.16E-01 2.000E+26 -5.430 2725.0 / PLOG / 1.00E+00 6.130E+28 -5.890 3154.0 / PLOG / 3.16E+00 2.140E+29 -5.800 3520.0 / PLOG / 1.00E+01 3.480E+28 -5.370 3636.0 / PLOG / 3.16E+01 3.320E+27 -4.950 3610.0 / PLOG / 1.00E+02 1.030E+27 -4.720 3680.0 / DUP C2H3+O2=CHCHO+OH 2.840E+14 -0.800 7232.0 PLOG / 1.00E-02 3.910E+11 -0.110 2131.0 / PLOG / 1.00E-01 1.130E+09 0.550 46.0 / PLOG / 3.16E-01 8.460E+08 0.560 1.0 / PLOG / 1.00E+00 2.750E+14 -1.830 5.0 / PLOG / 3.16E+00 2.580E+20 -2.840 7530.0 / PLOG / 1.00E+01 9.180E+14 -2.260 0.0 / PLOG / 3.16E+01 6.110E+25 -4.210 13050.0 / PLOG / 1.00E+02 1.650E+30 -5.350 18430.0 / DUP C2H3+O2=CHCHO+OH 2.840E+14 -0.800 7232.0 PLOG / 1.00E-02 9.910E+11 -0.660 -1.0 / PLOG / 1.00E-01 6.940E+14 -1.160 4542.0 / PLOG

/ 3.16E-01 2.790E+13 -0.720 3479.0 / PLOG / 1.00E+00 4.990E+11 -0.140 1995.0 / PLOG / 3.16E+00 2.350E+10 0.230 1573.0 / PLOG / 1.00E+01 1.700E+14 -0.820 4450.0 / PLOG / 3.16E+01 1.420E+11 0.050 3774.0 / PLOG / 1.00E+02 3.170E+11 -0.020 5338.0 / DUP

C2H3+O2=CH2CHO+O 1.760E+12 0.150 4205.0 PLOG / 1.00E-02 7.880E+20 -2.670 6742.0 / PLOG / 1.00E-01 7.720E+20 -2.670 6713.0 / PLOG / 3.16E-01 9.870E+20 -2.700 6724.0 / PLOG / 1.00E+00 7.100E+20 -2.650 6489.0 / PLOG / 3.16E+00 4.500E+20 -2.530 6406.0 / PLOG / 1.00E+01 1.760E+23 -3.220 8697.0 / PLOG / 3.16E+01 3.140E+25 -3.770 11530.0 / PLOG / 1.00E+02 1.020E+26 -3.800 13910.0 / DUP C2H3+O2=CH2CHO+O 1.760E+12 0.150 4205.0 PLOG / 1.00E-02 1.360E+10 0.620 -278.0 / PLOG / 1.00E-01 1.420E+10 0.620 -248.0 / PLOG / 3.16E-01 1.660E+10 0.600 -162.0 / PLOG / 1.00E+00 2.020E+10 0.580 38.0 / PLOG / 3.16E+00 9.750E+09 0.670 248.0 / PLOG / 1.00E+01 7.340E+09 0.720 778.0 / PLOG / 3.16E+01 1.570E+09 0.920 1219.0 / PLOG / 1.00E+02 7.850E+07 1.280 1401.0 / C2H3+O2=CH2CHO+O 1.760E+12 0.150 4205.0 PLOG / 1.00E-02 7.880E+20 -2.670 6742.0 / PLOG / 1.00E-01 7.720E+20 -2.670 6713.0 / PLOG / 3.16E-01 9.870E+20 -2.700 6724.0 / PLOG / 1.00E+00 7.100E+20 -2.650 6489.0 / PLOG / 3.16E+00 4.500E+20 -2.530 6406.0 / PLOG / 1.00E+01 1.760E+23 -3.220 8697.0 / PLOG / 3.16E+01 3.140E+25 -3.770 11530.0 / PLOG / 1.00E+02 1.020E+26 -3.800 13910.0 / DUP C2H3+O2=CH2CHO+O 1.760E+12 0.150 4205.0 PLOG / 1.00E-02 1.360E+10 0.620 -278.0 / PLOG / 1.00E-01 1.420E+10 0.620 -248.0 / PLOG / 3.16E-01 1.660E+10 0.600 -162.0 / PLOG / 1.00E+00 2.020E+10 0.580 38.0 / PLOG / 3.16E+00 9.750E+09 0.670 248.0 / PLOG / 1.00E+01 7.340E+09 0.720 778.0 / PLOG / 3.16E+01 1.570E+09 0.920 1219.0 / PLOG / 1.00E+02 7.850E+07 1.280 1401.0 / DUP

C2H3+O2=C2H2+HO2 6.490E+06 1.500 5218.0 PLOG / 1.00E-02 1.080E+07 1.280 3322.0 / PLOG / 1.00E-01 7.750E+06 1.330 3216.0 / PLOG / 3.16E-01 1.210E+07 1.270 3311.0 / PLOG / 1.00E+00 2.150E+07 1.190 3367.0 / PLOG / 3.16E+00 1.130E+08 1.000 3695.0 / PLOG / 1.00E+01 1.310E+11 0.120 5872.0 / PLOG / 3.16E+01 1.190E+09 0.820 5617.0 / PLOG / 1.00E+02 1.060E+17 -1.450 12230.0 / DUP C2H3+O2=C2H2+HO2 6.490E+06 1.500 5218.0 PLOG / 1.00E-02 4.760E+01 2.750 -796.0 / PLOG / 1.00E-01 5.160E+01 2.730 -768.0 / PLOG / 3.16E-01 5.550E+01 2.730 -658.0 / PLOG / 1.00E+00 4.600E+01 2.760 -493.0 / PLOG / 3.16E+00 3.750E+00 3.070 -601.0 / PLOG / 1.00E+01 5.480E+00 3.070 86.0 / PLOG / 3.16E+01 4.470E+08 0.000 955.0 / PLOG / 1.00E+02 2.020E+01 2.940 1847.0 / DUP

C2H3+O2=CHOCHO+H 3.080E+12 -0.260 3277.0 PLOG / 1.00E-02 4.790E+14 -1.030 912.0 / PLOG / 1.00E-01 5.030E+14 -1.040 922.0 / PLOG / 3.16E-01 6.430E+14 -1.070 983.0 / PLOG / 1.00E+00 3.730E+15 -1.290 1441.0 / PLOG / 3.16E+00 2.440E+18 -2.130 3234.0 / PLOG / 1.00E+01 1.300E+15 -1.090 2393.0 / PLOG / 3.16E+01 3.570E+33 -6.500 14910.0 / PLOG /

1.00E+02 3.280E+31 -5.760 16250.0 / DUP C2H3+O2=CHOCHO+H 3.080E+12 -0.260 3277.0 PLOG / 1.00E-02 2.800E-04 4.040 -7019.0 / PLOG / 1.00E-01 3.450E-04 4.010 -6978.0 / PLOG / 3.16E-01 9.730E-04 3.890 -6768.0 / PLOG / 1.00E+00 4.980E-01 3.150 -5496.0 / PLOG / 3.16E+00 1.340E+05 1.670 -2931.0 / PLOG / 1.00E+01 4.500E+15 -3.080 -4836.0 / PLOG / 3.16E+01 3.840E+10 0.220 941.0 / PLOG / 1.00E+02 2.750E+08 0.830 858.0 / DUP

C2H3+O2=CH2CO+OH 1.170E+03 2.430 7074.0 PLOG / 1.00E-02 8.660E+02 2.410 6061.0 / PLOG / 1.00E-01 8.910E+02 2.410 6078.0 / PLOG / 3.16E-01 9.430E+02 2.400 6112.0 / PLOG / 1.00E+00 1.060E+03 2.390 6180.0 / PLOG / 3.16E+00 1.090E+03 2.380 6179.0 / PLOG / 1.00E+01 1.390E+03 2.360 6074.0 / PLOG / 3.16E+01 2.490E+06 1.420 8480.0 / PLOG / 1.00E+02 1.660E+10 0.360 12010.0 / DUP C2H3+O2=CH2CO+OH 1.170E+03 2.430 7074.0 PLOG / 1.00E-02 1.820E-01 3.120 1331.0 / PLOG / 1.00E-01 2.070E-01 3.110 1383.0 / PLOG / 3.16E-01 2.710E-01 3.080 1496.0 / PLOG / 1.00E+00 5.260E-01 3.010 1777.0 / PLOG / 3.16E+00 1.370E+00 2.900 2225.0 / PLOG / 1.00E+01 4.190E-01 2.930 2052.0 / PLOG / 3.16E+01 1.190E-04 4.210 2043.0 / PLOG / 1.00E+02 1.300E-03 3.970 3414.0 / DUP

C2H3+O2=CH2O+HCO 1.160E+16 -1.130 3791.0 PLOG / 1.00E-02 2.490E+36 -7.600 12640.0 / PLOG / 1.00E-01 2.430E+36 -7.600 12610.0 / PLOG / 3.16E-01 1.950E+36 -7.570 12490.0 / PLOG / 1.00E+00 2.730E+35 -7.320 11820.0 / PLOG / 3.16E+00 1.430E+36 -7.470 12460.0 / PLOG / 1.00E+01 5.180E+35 -7.200 13430.0 / PLOG / 3.16E+01 3.190E+20 -2.570 5578.0 / PLOG / 1.00E+02 2.730E+33 -6.280 16000.0 / DUP C2H3+O2=CH2O+HCO 1.160E+16 -1.130 3791.0 PLOG / 1.00E-02 4.540E+15 -1.280 515.0 / PLOG / 1.00E-01 4.590E+15 -1.280 513.0 / PLOG / 3.16E-01 4.810E+15 -1.290 521.0 / PLOG / 1.00E+00 6.080E+15 -1.310 646.0 / PLOG / 3.16E+00 9.450E+15 -1.360 1066.0 / PLOG / 1.00E+01 2.560E+15 -1.180 1429.0 / PLOG / 3.16E+01 1.030E+69 -19.230 14760.0 / PLOG / 1.00E+02 4.210E+10 0.190 831.0 / DUP C2H3+O2=¿CH2O+H+CO 1.160E+16 -1.130 3791.0 PLOG / 1.00E-02 5.820E+36 -7.600 12640.0 / PLOG / 1.00E-01 5.660E+36 -7.600 12610.0 / PLOG / 3.16E-01 4.550E+36 -7.570 12490.0 / PLOG / 1.00E+00 6.360E+35 -7.320 11820.0 / PLOG / 3.16E+00 3.350E+36 -7.470 12460.0 / PLOG / 1.00E+01 1.210E+36 -7.200 13430.0 / PLOG / 3.16E+01 7.430E+20 -2.570 5578.0 / PLOG / 1.00E+02 6.360E+33 -6.280 16000.0 / DUP C2H3+O2=¿CH2O+H+CO 1.160E+16 -1.130 3791.0 PLOG / 1.00E-02 1.060E+16 -1.280 515.0 / PLOG / 1.00E-01 1.070E+16 -1.280 513.0 / PLOG / 3.16E-01 1.130E+16 -1.290 521.0 / PLOG / 1.00E+00 1.420E+16 -1.310 646.0 / PLOG / 3.16E+00 2.200E+16 -1.360 1066.0 / PLOG / 1.00E+01 5.980E+15 -1.180 1429.0 / PLOG / 3.16E+01 2.390E+69 -19.230 14760.0 / PLOG / 1.00E+02 9.810E+10 0.190 831.0 / DUP

C2H3+O2=CO+CH3O 3.090E+13 -0.890 3682.0 PLOG / 1.00E-02 8.190E+18 -2.660 3201.0 / PLOG / 1.00E-01 4.060E+14 -1.320 886.0 / PLOG / 3.16E-01 4.340E+14 -1.330 901.0 / PLOG

/ 1.00E+00 1.030E+11 -0.330 -748.0 / PLOG / 3.16E+00 1.890E+12 -3.000 -8995.0 / PLOG / 1.00E+01 1.930E+24 -5.630 2.0 / PLOG / 3.16E+01 1.100E+18 -2.220 5178.0 / PLOG / 1.00E+02 5.790E+32 -6.450 16810.0 / DUP C2H3+O2=CO+CH3O 3.090E+13 -0.890 3682.0 PLOG / 1.00E-02 1.290E+09 0.180 -1717.0 / PLOG / 1.00E-01 5.990E+11 -2.930 -9564.0 / PLOG / 3.16E-01 2.910E+11 -2.930 -10120.0 / PLOG / 1.00E+00 5.770E+21 -3.540 4772.0 / PLOG / 3.16E+00 4.990E+15 -1.620 1849.0 / PLOG / 1.00E+01 9.330E+16 -1.960 3324.0 / PLOG / 3.16E+01 1.020E+72 -20.690 15860.0 / PLOG / 1.00E+02 1.100E+09 0.310 1024.0 / DUP

C2H3+O2=CO2+CH3 6.160E+13 -1.050 3743.0 PLOG / 1.00E-02 2.370E+35 -7.760 12630.0 / PLOG / 1.00E-01 1.730E+35 -7.720 12520.0 / PLOG / 3.16E-01 4.470E+34 -7.550 12140.0 / PLOG / 1.00E+00 7.250E+31 -6.700 10440.0 / PLOG / 3.16E+00 3.630E+35 -7.750 12830.0 / PLOG / 1.00E+01 2.090E+35 -7.530 14050.0 / PLOG / 3.16E+01 3.840E+18 -2.440 5408.0 / PLOG / 1.00E+02 1.210E+32 -6.320 16190.0 / DUP C2H3+O2=CO2+CH3 6.160E+13 -1.050 3743.0 PLOG / 1.00E-02 6.270E+13 -1.160 406.0 / PLOG / 1.00E-01 6.240E+13 -1.160 401.0 / PLOG / 3.16E-01 6.120E+13 -1.160 397.0 / PLOG / 1.00E+00 5.320E+13 -1.140 447.0 / PLOG / 3.16E+00 1.450E+14 -1.260 988.0 / PLOG / 1.00E+01 5.020E+13 -1.110 1409.0 / PLOG / 3.16E+01 1.400E+70 -20.110 15430.0 / PLOG / 1.00E+02 9.210E+08 0.250 855.0 / DUP

C2H3OO=CHCHO+OH 5.890E+36 -7.100 51440.0 PLOG / 1.00E-02 3.640E+49 -12.130 67420.0 / PLOG / 1.00E-01 1.440E+36 -9.920 41220.0 / PLOG / 3.16E-01 4.180E+40 -10.530 43670.0 / PLOG / 1.00E+00 3.790E+46 -10.720 51900.0 / PLOG / 3.16E+00 1.600E+49 -11.240 54150.0 / PLOG / 1.00E+01 2.380E+51 -11.640 56980.0 / PLOG / 3.16E+01 2.000E+54 -12.220 61840.0 / PLOG / 1.00E+02 9.540E+195 -52.270 163500.0 / DUP C2H3OO=CHCHO+OH 5.890E+36 -7.100 51440.0 PLOG / 1.00E-02 1.170E+56 -14.810 60700.0 / PLOG / 1.00E-01 2.320E+40 -9.390 50420.0 / PLOG / 3.16E-01 1.610E+43 -9.990 50290.0 / PLOG / 1.00E+00 2.330E+124 -36.770 70100.0 / PLOG / 3.16E+00 1.880E+103 -29.490 65410.0 / PLOG / 1.00E+01 5.960E+86 -23.810 62170.0 / PLOG / 3.16E+01 1.510E+57 -13.940 55390.0 / PLOG / 1.00E+02 1.790E+34 -6.400 50000.0 / DUP

C2H3OO=CH2CHO+O 1.220E+29 -4.710 42340.0 PLOG / 1.00E-02 2.700E+180 -48.190 169300.0 / PLOG / 1.00E-01 3.900E+38 -8.690 42770.0 / PLOG / 3.16E-01 4.570E+47 -11.210 47050.0 / PLOG / 1.00E+00 7.620E+81 -21.280 65080.0 / PLOG / 3.16E+00 1.860E+68 -16.830 60680.0 / PLOG / 1.00E+01 2.020E+55 -12.690 55840.0 / PLOG / 3.16E+01 1.110E+53 -11.790 56690.0 / PLOG / 1.00E+02 4.300E+48 -10.310 56090.0 / DUP C2H3OO=CH2CHO+O 1.220E+29 -4.710 42340.0 PLOG / 1.00E-02 1.470E+30 -6.640 41110.0 / PLOG / 1.00E-01 9.650E-12 5.960 22890.0 / PLOG / 3.16E-01 3.950E+22 -3.710 36270.0 / PLOG / 1.00E+00 2.390E+33 -6.620 41280.0 / PLOG / 3.16E+00 6.370E+31 -5.960 41260.0 / PLOG / 1.00E+01 2.130E+29

-5.100 40710.0 / PLOG / 3.16E+01 4.660E+27 -4.500 40530.0 / PLOG / 1.00E+02 5.990E+25 -3.850 40120.0 / DUP

C2H3OO=CHOCHO+H 4.720E+20 -2.690 32320.0 PLOG / 1.00E-02 6.410E+80 -22.200 51750.0 / PLOG / 1.00E-01 3.310E+65 -17.010 48090.0 / PLOG / 3.16E-01 5.980E+51 -12.620 43000.0 / PLOG / 1.00E+00 1.480E+44 -10.120 40790.0 / PLOG / 3.16E+00 1.260E+59 -14.330 51390.0 / PLOG / 1.00E+01 4.930E+26 -4.670 34320.0 / PLOG / 3.16E+01 2.060E+33 -6.380 39520.0 / PLOG / 1.00E+02 1.300E+32 -5.920 40660.0 / DUP C2H3OO=CHOCHO+H 4.720E+20 -2.690 32320.0 PLOG / 1.00E-02 1.190E+28 -6.010 28740.0 / PLOG / 1.00E-01 1.400E+25 -4.800 28940.0 / PLOG / 3.16E-01 2.910E+20 -3.290 27550.0 / PLOG / 1.00E+00 1.580E+19 -2.820 27620.0 / PLOG / 3.16E+00 1.930E+22 -3.540 29980.0 / PLOG / 1.00E+01 7.510E+29 -5.750 34490.0 / PLOG / 3.16E+01 7.140E+61 -16.160 43280.0 / PLOG / 1.00E+02 1.140E+19 -2.560 29670.0 / DUP

C2H3OO=CH2CO+OH 1.550E+24 -3.870 49850.0 PLOG / 1.00E-02 1.150E+47 -12.280 75330.0 / PLOG / 1.00E-01 8.430E+09 -2.060 33720.0 / PLOG / 3.16E-01 6.060E+04 0.170 34220.0 / PLOG / 1.00E+00 1.510E+19 -3.610 43060.0 / PLOG / 3.16E+00 2.130E+33 -7.390 51610.0 / PLOG / 1.00E+01 4.440E+36 -7.990 54680.0 / PLOG / 3.16E+01 1.190E+37 -7.800 56460.0 / PLOG / 1.00E+02 9.080E+35 -7.210 57550.0 / DUP C2H3OO=CH2CO+OH 1.550E+24 -3.870 49850.0 PLOG / 1.00E-02 2.310E+02 -0.730 25710.0 / PLOG / 1.00E-01 1.830E-23 7.840 20190.0 / PLOG / 3.16E-01 3.820E+63 -20.440 43420.0 / PLOG / 1.00E+00 3.180E+27 -7.760 37230.0 / PLOG / 3.16E+00 2.320E-05 3.470 31560.0 / PLOG / 1.00E+01 1.060E-01 2.640 34160.0 / PLOG / 3.16E+01 5.620E+02 1.700 36450.0 / PLOG / 1.00E+02 1.110E+07 0.520 38670.0 / DUP

C2H3OO=CH2O+HCO 1.190E+20 -2.290 30170.0 PLOG / 1.00E-02 1.660E+174 -55.520 60320.0 / PLOG / 1.00E-01 9.030E+66 -17.250 48120.0 / PLOG / 3.16E-01 1.820E+43 -9.870 37960.0 / PLOG / 1.00E+00 8.640E+33 -6.880 34370.0 / PLOG / 3.16E+00 7.290E+171 -43.530 191900.0 / PLOG / 1.00E+01 1.030E+32 -6.060 35500.0 / PLOG / 3.16E+01 1.850E+34 -6.570 38510.0 / PLOG / 1.00E+02 5.700E+29 -5.190 36800.0 / DUP C2H3OO=CH2O+HCO 1.190E+20 -2.290 30170.0 PLOG / 1.00E-02 2.270E+35 -7.970 31280.0 / PLOG / 1.00E-01 2.080E+26 -4.960 28780.0 / PLOG / 3.16E-01 1.450E+20 -3.080 26630.0 / PLOG / 1.00E+00 1.060E+130 -39.380 54700.0 / PLOG / 3.16E+00 2.350E+34 -6.870 35700.0 / PLOG / 1.00E+01 2.180E+175 -53.780 68500.0 / PLOG / 3.16E+01 1.070E+185 -54.220 88990.0 / PLOG / 1.00E+02 4.680E+02 1.810 18100.0 / DUP

C2H3OO=¿CH2O+H+CO 1.190E+20 -2.290 30170.0 PLOG / 1.00E-02 3.880E+174 -55.520 60320.0 / PLOG / 1.00E-01 2.110E+67 -17.250 48120.0 / PLOG / 3.16E-01 4.260E+43 -9.870 37960.0 / PLOG / 1.00E+00 2.020E+34 -6.880 34370.0 / PLOG / 3.16E+00 1.700E+172 -

43.530 191900.0 / PLOG / 1.00E+01 2.400E+32 -6.060 35500.0 / PLOG / 3.16E+01 4.320E+34 -6.570 38510.0 / PLOG / 1.00E+02 1.330E+30 -5.190 36800.0 / DUP C2H3OO=¿CH2O+H+CO 1.190E+20 -2.290 30170.0 PLOG / 1.00E-02 5.290E+35 -7.970 31280.0 / PLOG / 1.00E-01 4.850E+26 -4.960 28780.0 / PLOG / 3.16E-01 3.370E+20 -3.080 26630.0 / PLOG / 1.00E+00 2.460E+130 -39.380 54700.0 / PLOG / 3.16E+00 5.490E+34 -6.870 35700.0 / PLOG / 1.00E+01 5.090E+175 -53.780 68500.0 / PLOG / 3.16E+01 2.490E+185 -54.220 88990.0 / PLOG / 1.00E+02 1.090E+03 1.810 18100.0 / DUP C2H3OO=CO+CH3O 1.160E-01 3.160 18420.0 PLOG / 1.00E-02 5.200E+33 -7.920 31320.0 / PLOG / 1.00E-01 1.260E+98 -27.090 64060.0 / PLOG / 3.16E-01 1.800E+33 -7.270 33760.0 / PLOG / 1.00E+00 3.830E+33 -7.200 35100.0 / PLOG / 3.16E+00 1.280E+79 -19.610 74870.0 / PLOG / 1.00E+01 4.070E+32 -6.620 37210.0 / PLOG / 3.16E+01 6.860E+44 -10.040 47030.0 / PLOG / 1.00E+02 1.000E-10 0.000 0.0 / DUP C2H3OO=CO+CH3O 1.160E-01 3.160 18420.0 PLOG / 1.00E-02 2.310E+129 -41.860 45850.0 / PLOG / 1.00E-01 2.420E+28 -5.990 30540.0 / PLOG / 3.16E-01 8.690E-50 16.630 -3900.0 / PLOG / 1.00E+00 1.190E-39 13.610 -1317.0 / PLOG / 3.16E+00 8.800E+86 -23.080 61010.0 / PLOG / 1.00E+01 1.270E+03 1.440 18660.0 / PLOG / 3.16E+01 1.970E+17 -2.230 28590.0 / PLOG / 1.00E+02 3.250E+04 1.694 23328.0 / DUP CHOCHO+OH=¿HCO+CO+H2O 6.130E+04 2.650 -4586.0 C2H3+H=C2H2+H2 1.700E+14 0.000 0.0 C2H3+H=H2CC+H2 6.000E+13 0.000 0.0 C2H3+OH=C2H2+H2O 3.010E+13 0.000 0.0 C2H3+CH3=CH4+C2H2 3.920E+11 0.000 0.0 C2H3+C2H3=C2H2+C2H4 9.600E+11 0.000 0.0 C2H+H(+M)=C2H2(+M) 1.000E+17 0.000 0.0 LOW / 3.750E+33 -4.800 1900.0 / TROE / 6.460E-01 1.320E+02 1.315E+03 5.566E+03 / H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ C2H2(+M)=H2CC(+M) 8.000E+14 -0.520 50750.0 LOW / 2.450E+15 -0.640 49700.0 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/ 2.50/ C2H4/ 2.50/ C2H2+O=CH2+CO 7.400E+08 1.280 2472.0 C2H2+O=HCCO+H 2.960E+09 1.280 2472.0 C2H2+HO2=CH2CO+OH 6.030E+09 0.000 7949.0 C2H2+HCO=C2H3+CO 1.000E+07 2.000 6000.0 C2H2+CH2=C3H3+H 1.200E+13 0.000 6620.0 C2H2+CH2(S)=C3H3+H 2.000E+13 0.000 0.0 C2H2+HCCO=C3H3+CO 1.000E+11 0.000 3000.0

H2CC+H=C2H2+H 1.000E+14 0.000 0.0 H2CC+OH=CH2CO+H 2.000E+13 0.000 0.0 H2CC+O2=HCO+HC 1.000E+13 0.000 0.0 C2H2+OH=C2H+H2O 2.630E+06 2.140 17060.0 C2H2+OH=HCCOH+H 2.800E+05 2.280 12420.0 PLOG / 1.00E-02 2.800E+05 2.280 12420.0 / PLOG / 2.50E-02 7.470E+05 2.160 12550.0 / PLOG / 1.00E-01 1.780E+06 2.040 12670.0 / PLOG / 1.00E+00 2.420E+06 2.000 12710.0 / PLOG / 1.00E+01 3.210E+06 1.970 12810.0 / PLOG / 1.00E+02 7.350E+06 1.890 13600.0 / C2H2+OH=CH2CO+H 1.580E+03 2.560 -844.0 PLOG / 1.00E-02 1.580E+03 2.560 -844.0 / PLOG / 2.50E-02 1.520E+04 2.280 -292.0 / PLOG / 1.00E-01 3.020E+05 1.920 598.0 / PLOG / 1.00E+00 7.530E+06 1.550 2106.0 / PLOG / 1.00E+01 5.100E+06 1.650 3400.0 / PLOG / 1.00E+02 1.460E+04 2.450 4477.0 / C2H2+OH=CH3+CO 4.760E+05 1.680 -330.0 PLOG /

1.00E-02 4.760E+05 1.680 -330.0 / PLOG / 2.50E-02 4.370E+06 1.400 226.0 / PLOG / 1.00E-01 7.650E+07 1.050 1115.0 / PLOG / 1.00E+00 1.280E+09 0.730 2579.0 / PLOG / 1.00E+01 4.310E+08 0.920 3736.0 / PLOG / 1.00E+02 8.250E+05 1.770 4697.0 / C2H2+OH=C2H2OH 3.910E+32 -7.126 5824.0 PLOG / 1.00E-02 3.910E+32 -7.126 5824.0 / PLOG / 2.50E-02 1.070E+32 -6.847 5508.0 / PLOG / 1.00E-01 1.650E+32 -6.717 5822.0 / PLOG / 1.00E+00 1.390E+31 -6.087 6348.0 / PLOG / 1.00E+01 2.890E+29 -5.288 7055.0 / PLOG / 1.00E+02 1.370E+25 -3.754 6543.0 / H+HCCOH=H+CH2CO 1.000E+13 0.000 0.0 C2H+O2=CO2+CHV 2.170E+10 0.000 0.0 C2H+O2=HCO+CO 5.000E+13 0.000 1500.0 C2H+O=CO+CHV 6.200E+12 0.000 0.0 C2H+O=CO+CH 5.000E+13 0.000 0.0 C2H+H2=H+C2H2 4.900E+05 2.500 560.0 C2H+OH=H+HCCO 2.000E+13 0.000 0.0 CH3CHO(+M)=CH3+HCO(+M) 2.450E+22 -1.740 86355.0 LOW / 1.030E+59 -11.300 95912.0 / TROE / 2.490E-03 7.181E+02 6.089E+00 3.780E+03 / CH3CHO(+M)=CH4+CO(+M) 2.720E+21 -1.740 86355.0 LOW / 1.140E+58 -11.300 95912.0 / TROE / 2.490E-03 7.181E+02 6.089E+00 3.780E+03 / CH3CHO+O2=CH3CO+HO2 3.010E+13 0.000 39150.0 CH3CHO+O=CH3CO+OH 5.940E+12 0.000 1868.0 CH3CHO+H=CH3CO+H2 1.310E+05 2.580 1220.0 CH3CHO+OH=CH3CO+H2O 3.370E+12 0.000 -619.0 CH3CHO+HO2=CH3CO+H2O2 3.010E+12 0.000 11920.0 CH3CHO+CH3=CH3CO+CH4 7.080E-04 4.580 1966.0 CH3CHO+CH3O2=CH3CO+CH3O2H 3.010E+12 0.000 11920.0 CH3CHO+CH3CO3=CH3 3.010E+12 0.000 11920.0 CH3CHO+H=CH2CHO+H2 2.720E+03 3.100 5210.0 CH3CHO+OH=CH2CHO+H2O 1.720E+05 2.400 815.0 CH3CHO+OH=CH3+HOCHO 3.000E+15 -1.076 0.0 CH3CO(+M)=CH3+CO(+M) 1.070E+12 0.630 16900.0 LOW / 5.650E+18 -0.970 14600.0 / TROE / 6.290E-01 8.730E+09 5.520E+00 7.600E+07 / CH3CO(+M)=CH2CO+H(+M) 9.410E+07 1.917 44987.0 LOW / 1.520E+51 -10.270 55390.0 / TROE / 6.009E-01 8.103E+09 6.677E+02 5.000E+09 / CH3CO+H=CH2CO+H2 2.000E+13 0.000 0.0 CH3CO+O=CH2CO+OH 2.000E+13 0.000 0.0 CH3CO+CH3=CH2CO+CH4 5.000E+13 0.000 0.0 CH3CO+O2=CH3CO3 1.200E+11 0.000 -1100.0 CH3CO3+HO2=CH3CO3H+O2 1.750E+10 0.000 -3275.0 H2O2+CH3CO3=HO2+CH3CO3H 2.410E+12 0.000 9936.0 CH4+CH3CO3=CH3+CH3C 1.810E+11 0.000 18480.0 C2H3OH=CH3CHO 7.420E+46 -10.560 67420.0 PLOG / 1.00E-01 7.420E+46 -10.560 67420.0 / PLOG / 1.00E+00 4.420E+42 -9.090 67069.0 / PLOG / 1.00E+02 2.900E+27 -4.350 61613.0 / C2H3OH+O2=CH2CHO+HO2 5.310E+11 0.210 39830.0 C2H3OH+O=CH2CHO+OH 1.880E+06 1.900 -860.0 C2H3OH+H=CH2CHO+H2 1.480E+03 3.077 7220.0 C2H3OH+OH=CH2CHO+H2O 3.330E+09 1.100 540.0 C2H3OH+CH3=CH2CHO+CH4 2.030E-08 5.900 1052.0 C2H3OH+CH3O2=CH2CHO+CH 3.400E+03 2.500 8922.0 C2H3OH+H=C2H2OH+H2 2.470E+07 2.030 15200.0 C2H3OH+H=PC2H4OH 3.010E+08 1.577 3670.0 C2H3OH+HO2=CH3CHO+HO2 1.490E+05 1.670 6810.0 CH2CHO(+M)=CH2CO+H(+M 1.430E+15 -0.150 45600.0 LOW / 6.000E+29 -3.800 43424.0 / TROE / 9.850E-01 3.930E+02 9.800E+09 5.000E+09 / CH2CHO(+M)=CH3+CO(+M) 2.930E+12 0.290 40300.0 LOW / 9.520E+33 -5.070 41300.0 / TROE / 7.130E-17 1.150E+03 4.990E+09 1.790E+09 /

SC2H4OH=CH3CHO+H 5.690E+52 -13.380 45049.0 PLOG / 1.00E-03 5.690E+52 -13.380

45049.0 / PLOG / 1.00E-02 3.290E+56 -14.120 48129.0 / PLOG / 1.00E-01 8.580E+57 -14.160
50743.0 / PLOG / 1.00E+00 5.360E+55 -13.150 51886.0 / PLOG / 1.00E+01 1.660E+48 -10.640
50297.0 / PLOG / 2.00E+01 8.260E+44 -9.590 49218.0 / PLOG / 5.00E+01 1.010E+40 -8.060
47439.0 / PLOG / 1.00E+02 1.100E+36 -6.840 45899.0 / SC2H4OH=C2H3OH+H 5.400E+46
-11.630 44323.0 PLOG / 1.00E-03 5.400E+46 -11.630 44323.0 / PLOG / 1.00E-02 1.210E+51
-12.550 47240.0 / PLOG / 1.00E-01 2.870E+54 -13.150 50702.0 / PLOG / 1.00E+00 3.790E+53
-12.510 52560.0 / PLOG / 1.00E+01 6.330E+46 -10.200 51441.0 / PLOG / 2.00E+01 3.870E+43
-9.170 50440.0 / PLOG / 5.00E+01 5.080E+38 -7.650 48713.0 / PLOG / 1.00E+02 5.120E+34
-6.410 47182.0 / SC2H4OH=C2H5O 5.480E+45 -11.630 44328.0 PLOG / 1.00E-03 5.480E+45
-11.630 44328.0 / PLOG / 1.00E-02 2.540E+49 -12.370 46445.0 / PLOG / 1.00E-01 1.650E+54
-13.400 50330.0 / PLOG / 1.00E+00 1.810E+55 -13.310 53132.0 / PLOG / 1.00E+01 4.580E+49
-11.320 52714.0 / PLOG / 2.00E+01 4.110E+46 -10.330 51834.0 / PLOG / 5.00E+01 6.680E+41
-8.830 50202.0 / PLOG / 1.00E+02 6.540E+37 -7.580 48697.0 / SC2H4OH=PC2H4OH 2.650E+36
-8.860 51019.0 PLOG / 1.00E-03 2.650E+36 -8.860 51019.0 / PLOG / 1.00E-02 3.560E+37 -
8.890 51114.0 / PLOG / 1.00E-01 4.140E+39 -9.190 51912.0 / PLOG / 1.00E+00 5.820E+44
-10.340 55296.0 / PLOG / 1.00E+01 4.260E+48 -11.060 59458.0 / PLOG / 2.00E+01 8.840E+47
-10.740 59901.0 / PLOG / 5.00E+01 2.230E+45 -9.840 59604.0 / PLOG / 1.00E+02 1.700E+42
-8.830 58737.0 / CH3+CH2O=C2H5O 3.000E+11 0.000 6336.0 CH3CHO+H=C2H5O 4.610E+07
1.710 7090.0 C2H5O+O2=CH3CHO+HO2 4.280E+10 0.000 1097.0 O2C2H4OH=PC2H4OH+O2
3.900E+16 -1.000 30000.0 O2C2H4OH=¿OH+CH2O+CH2O 1.250E+11 0.000 18900.0 SC2H4OH+O2=CH3CHO-
5.260E+17 -1.638 869.0 PLOG / 1.00E-02 5.260E+17 -1.637 838.0 / PLOG / 1.00E-01 5.260E+17
-1.637 838.0 / PLOG / 1.00E+00 5.280E+17 -1.638 839.0 / PLOG / 1.00E+01 1.540E+18 -
1.771 1120.0 / PLOG / 1.00E+02 3.780E+20 -2.429 3090.0 / SC2H4OH+O2=C2H3OH+HO2
5.510E+03 2.495 -414.0 PLOG / 1.00E-02 5.120E+02 2.496 -414.0 / PLOG / 1.00E-01 5.330E+02
2.490 -402.0 / PLOG / 1.00E+00 7.620E+02 2.446 -296.0 / PLOG / 1.00E+01 8.920E+03
2.146 470.0 / PLOG / 1.00E+02 4.380E+05 1.699 2330.0 / CH3OCH3(+M)=CH3+CH3O(+M)
2.330E+19 -0.661 84139.0 LOW / 1.720E+59 -11.400 93296.0 / TROE / 1.000E+00 1.000E-30
8.800E+02 / H2/ 3.00/ CO/ 2.25/ CO2/ 3.00/ N2/ 1.50/ H2O/ 9.00/ CH3OCH3/ 5.00/ CH4/
3.00/ C2H6/ 4.50/ CH3OCH3+OH=CH3OCH2+H2O 9.350E+05 2.290 -781.0 CH3OCH3+H=CH3OCH2+H2
7.720E+06 2.090 3384.0 CH3OCH3+O=CH3OCH2+OH 7.750E+08 1.360 2250.0 CH3OCH3+HO2=CH3OCH2+H
3.170E-03 4.640 10556.0 CH3OCH3+CH3O2=CH3OCH2+CH3O2H 1.270E-03 4.640 10556.0 CH3OCH3+CH3=CH
7.020E+00 3.780 9687.0 CH3OCH3+O2=CH3OCH2+HO2 4.100E+13 0.000 44910.0 CH3OCH3+CH3O=CH3OCH
6.020E+11 0.000 4074.0 CH3OCH3+CH3OCH2O2=CH3OCH2+CH3OCH2O2H 5.000E+12 0.000
17690.0 CH3OCH3+O2CHO=CH3OCH2+HO2CHO 4.420E+04 2.600 13910.0 CH3OCH3+OCHO=CH3OCH2+HO
1.000E+13 0.000 17690.0 CH3OCH2+CH3O=CH3OCH3+CH2O 2.410E+13 0.000 0.0 CH3OCH2+CH2O=CH3OC
5.490E+03 2.800 5862.0 CH3OCH2+CH3CHO=CH3OCH3+CH3CO 1.260E+12 0.000 8499.0 CH3OCH2=CH3+CH

8.030E+12 0.440 26491.0 PLOG / 1.00E-02 7.490E+23 -4.515 25236.0 / PLOG / 1.00E-01 6.920E+28 -5.727 27495.0 / PLOG / 1.00E+00 4.230E+29 -5.610 28898.0 / PLOG / 1.00E+01 6.610E+27 -4.707 29735.0 / PLOG / 1.00E+02 2.660E+29 -4.936 31786.0 / CH3OCH2+O2=CH3OCH2O2 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.120E+18 -3.370 -4294.0 / PLOG / 1.00E-02 1.330E+21 -3.950 -2615.0 / PLOG / 1.00E+00 1.130E+28 -5.240 4088.0 / PLOG / 2.00E+00 3.910E+27 -5.000 4512.0 / PLOG / 1.00E+01 2.750E+24 -3.870 4290.0 / PLOG / 2.00E+01 2.970E+22 -3.230 3781.0 / PLOG / 5.00E+01 5.190E+19 -2.350 2908.0 / PLOG / 1.00E+02 5.430E+17 -1.730 2210.0 / CH3OCH2+O2=CH2OCH2O2H 1.000E+00 1.000 1.0 PLOG / 1.00E-03 5.080E+20 -4.390 469.0 / PLOG / 1.00E-02 5.470E+23 -4.960 2183.0 / PLOG / 1.00E+00 2.810E+28 -5.630 7848.0 / PLOG / 2.00E+00 5.190E+27 -5.330 8144.0 / PLOG / 1.00E+01 9.670E+24 -4.360 8417.0 / PLOG / 2.00E+01 4.080E+23 -3.900 8494.0 / PLOG / 5.00E+01 5.080E+21 -3.280 8585.0 / PLOG / 1.00E+02 1.620E+20 -2.810 8619.0 / CH3OCH2+O2=¿CH2O+CH2O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-03 8.010E+21 -3.180 3067.0 / PLOG / 1.00E-02 1.730E+23 -3.550 4050.0 / PLOG / 1.00E+00 2.040E+31 -5.760 11594.0 / PLOG / 2.00E+00 5.990E+31 -5.870 12710.0 / PLOG / 1.00E+01 9.390E+30 -5.590 14517.0 / PLOG / 2.00E+01 1.090E+30 -5.300 15051.0 / PLOG / 5.00E+01 3.580E+28 -4.880 15664.0 / PLOG / 1.00E+02 2.410E+27 -4.550 16107.0 / CH3OCH2O2=CH2OCH2O2H 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.940E+29 -6.990 22446.0 / PLOG / 1.00E-02 4.070E+27 -6.160 21619.0 / PLOG / 1.00E+00 2.520E+25 -4.760 22691.0 / PLOG / 2.00E+00 5.970E+24 -4.480 22868.0 / PLOG / 1.00E+01 4.440E+21 -3.380 22386.0 / PLOG / 2.00E+01 4.520E+19 -2.740 21803.0 / PLOG / 5.00E+01 5.720E+16 -1.820 20829.0 / PLOG / 1.00E+02 3.700E+14 -1.130 20034.0 / CH3OCH2O2=¿CH2O+CH2O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-03 2.060E+36 -8.320 33415.0 / PLOG / 1.00E-02 2.070E+39 -8.860 35842.0 / PLOG / 1.00E+00 1.120E+40 -8.420 39835.0 / PLOG / 2.00E+00 9.720E+38 -8.040 39923.0 / PLOG / 1.00E+01 6.280E+35 -6.970 39900.0 / PLOG / 2.00E+01 1.600E+34 -6.460 39850.0 / PLOG / 5.00E+01 8.320E+31 -5.750 39719.0 / PLOG / 1.00E+02 1.220E+30 -5.200 39549.0 / CH2OCH2O2H=¿CH2O+CH2O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.660E+23 -4.530 22243.0 / PLOG / 1.00E-02 5.300E+25 -4.930 24158.0 / PLOG / 1.00E+00 7.810E+22 -3.500 23156.0 / PLOG / 2.00E+00 4.980E+22 -3.350 23062.0 / PLOG / 1.00E+01 8.460E+22 -3.220 23559.0 / PLOG / 2.00E+01 9.090E+22 -3.140 23899.0 / PLOG / 5.00E+01 4.590E+22 -2.940 24262.0 / PLOG / 1.00E+02 1.400E+22 -2.720 24407.0 / CH2OCH2O2H+O2=O2CH2OCH2O2H 1.000E+00 1.000 1.0 PLOG / 1.00E-03 9.420E+12 -1.680 -4998.0 / PLOG / 1.00E-02 8.160E+16 -2.500 -2753.0 / PLOG / 1.00E+00 1.060E+22 -3.300 3389.0 / PLOG / 2.00E+00 3.480E+20 -2.790 3131.0 / PLOG / 1.00E+01 2.860E+16 -1.480 1873.0 / PLOG / 2.00E+01 8.550E+14 -1.010 1312.0 / PLOG / 5.00E+01 2.680E+13 -0.540 727.0 / PLOG / 1.00E+02 4.870E+12 -0.320 428.0 / CH2OCH2O2H+O2=HO2CH2OCHO+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-03 5.900E+20 -2.880 3234.0 / PLOG / 1.00E-02 2.060E+23 -3.590 5116.0 / PLOG / 1.00E+00 4.450E+29 -5.290

12791.0 / PLOG / 2.00E+00 2.440E+28 -4.920 12891.0 / PLOG / 1.00E+01 9.420E+23 -3.680
12049.0 / PLOG / 2.00E+01 1.040E+22 -3.160 11505.0 / PLOG / 5.00E+01 6.950E+19 -2.600
10861.0 / PLOG / 1.00E+02 3.960E+18 -2.310 10500.0 / O2CH2OCH2O2H=HO2CH2OCHO+OH
1.000E+00 1.000 1.0 PLOG / 1.00E-03 9.050E+23 -4.880 18805.0 / PLOG / 1.00E-02 6.840E+26
-5.320 22533.0 / PLOG / 1.00E+00 5.070E+16 -1.810 21175.0 / PLOG / 2.00E+00 2.660E+14
-1.110 20310.0 / PLOG / 1.00E+01 1.690E+10 0.180 18604.0 / PLOG / 2.00E+01 1.110E+09
0.540 18100.0 / PLOG / 5.00E+01 1.070E+08 0.840 17661.0 / PLOG / 1.00E+02 3.860E+07
0.980 17467.0 / CH3OCH2O2+CH3OCH2O2=¿O2+CH3OCH2O+CH3OCH2O 1.550E+23 -4.500
0.0 CH3OCH2O2+CH2O=CH3OCH2O2H+HCO 1.000E+12 0.000 11660.0 CH3OCH2O2+CH3CHO=CH3OCH2O2
2.800E+12 0.000 13600.0 CH3OCH2O+OH=CH3OCH2O2H 2.000E+13 0.000 0.0 HO2CH2OCHO=OCH2OCHO+
5.000E+16 0.000 43000.0 CH2O+OCHO=OCH2OCHO 1.250E+11 0.000 11900.0 OCH2OCHO=HOCH2OCO
1.000E+11 0.000 14000.0 HOCH2OCO=CH2OH+CO2 1.120E+17 -1.526 20772.0 HOCH2OCO=HOCH2O+CO
2.920E+18 -1.965 19619.0 CH3O+CH2O=CH3OCH2O 1.000E+11 0.000 7960.0 CH3OCH2O+O2=CH3OCHO+HO
4.380E-19 9.500 -5501.0 CH3OCH2O=CH3OCHO+H 3.300E+13 0.004 26136.0 CH3O+HCO=CH3OCHO
3.000E+13 0.000 0.0 CH3O+HCO=CH3OH+CO 9.000E+13 0.000 0.0 CH3+OCHO=CH3OCHO
1.000E+13 0.000 0.0 CH2OCHO+H=CH3OCHO 1.000E+14 0.000 0.0 CH3OCO+H=CH3OCHO
1.000E+14 0.000 0.0 CH3OCHO+O2=CH3OCO+HO2 1.000E+13 0.000 49700.0 CH3OCHO+O2=CH2OCHO+HO
2.050E+13 0.000 52000.0 CH3OCHO+OH=CH3OCO+H2O 1.580E+07 1.800 934.0 CH3OCHO+OH=CH2OCHO+
5.270E+09 0.970 1586.0 CH3OCHO+HO2=CH3OCO+H2O2 4.820E+03 2.600 13910.0 CH3OCHO+HO2=CH2OC
2.380E+04 2.550 16490.0 CH3OCHO+O=CH3OCO+OH 2.760E+05 2.450 2830.0 CH3OCHO+O=CH2OCHO+OH
9.800E+05 2.430 4750.0 CH3OCHO+H=CH3OCO+H2 6.500E+05 2.400 4471.0 CH3OCHO+H=CH2OCHO+H2
6.650E+05 2.540 6756.0 CH3OCHO+CH3=CH3OCO+CH4 7.550E-01 3.460 5481.0 CH3OCHO+CH3=CH2OCHO+
4.520E-01 3.650 7154.0 CH3OCHO+CH3O=CH3OCO+CH3OH 5.480E+11 0.000 5000.0 CH3OCHO+CH3O=CH2O
2.170E+11 0.000 6458.0 CH3OCHO+CH3O2=CH3OCO+CH3O2H 4.820E+03 2.600 13910.0 CH3OCHO+CH3O2=
2.380E+04 2.550 16490.0 CH3OCHO+HCO=CH3OCO+CH2O 5.400E+06 1.900 17010.0 CH3OCHO+HCO=CH2O
1.020E+05 2.500 18430.0 CH3OCO=CH2OCHO 1.630E+12 -0.180 40670.0 CH3OCO=CH3+CO2
8.690E+17 -1.810 13657.0 PLOG / 5.00E-02 9.720E+12 -1.310 9417.0 / PLOG / 1.00E+00
1.250E+16 -1.830 11341.0 / PLOG / 1.00E+01 1.040E+18 -2.100 12827.0 / PLOG / 1.00E+02
8.690E+17 -1.810 13657.0 / CH3OCO=CH3O+CO 8.690E+17 -1.810 13657.0 PLOG / 5.00E-
02 1.030E+03 1.290 25401.0 / PLOG / 1.00E+00 4.090E+05 0.810 21969.0 / PLOG / 1.00E+01
9.020E+14 -1.720 21768.0 / PLOG / 1.00E+02 2.830E+22 -3.440 23592.0 / CH2O+HCO=CH2OCHO
1.500E+11 0.000 11900.0 C3H8(+M)=CH3+C2H5(+M) 1.290E+37 -5.840 97380.0 LOW / 5.640E+74
-15.740 98714.0 / TROE / 3.100E-01 5.000E+01 3.000E+03 9.000E+03 / H2/ 2.00/ H2O/
6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/ HE/ 0.70/ NC3H7+H=C3H8
1.000E+14 0.000 0.0 IC3H7+H=C3H8 1.000E+14 0.000 0.0 C3H8+IC3H7=NC3H7+C3H8 3.000E+10
0.000 12900.0 C3H8+O2=IC3H7+HO2 2.000E+13 0.000 49640.0 C3H8+H=IC3H7+H2 1.300E+06

2.400 4471.0 C3H8+O=IC3H7+OH 5.490E+05 2.500 3140.0 C3H8+OH=IC3H7+H2O 4.670E+07
1.610 -35.0 C3H8+HO2=IC3H7+H2O2 6.320E+01 3.370 13720.0 C3H8+CH3=IC3H7+CH4 6.400E+04
2.170 7520.0 C3H8+C2H3=IC3H7+C2H4 1.000E+11 0.000 10400.0 C3H8+C2H5=IC3H7+C2H6
1.000E+11 0.000 10400.0 C3H8+C3H5-A=IC3H7+C3H6 7.940E+11 0.000 16200.0 C3H8+CH3O=IC3H7+CH3OH
3.000E+11 0.000 7000.0 C3H8+CH3O2=IC3H7+CH3O2H 1.020E+01 3.580 14810.0 C3H8+C2H5O2=IC3H7+C2H
1.020E+01 3.580 14810.0 C3H8+NC3H7O2=IC3H7+NC3H7O2H 2.000E+12 0.000 17000.0 C3H8+CH3CO3=IC3H
2.000E+12 0.000 17000.0 C3H8+O2CHO=IC3H7+HO2CHO 1.480E+04 2.600 13910.0 C3H8+IC3H7O2=IC3H7+I
2.000E+12 0.000 17000.0 C3H8+O2=NC3H7+HO2 6.000E+13 0.000 52290.0 C3H8+H=NC3H7+H2
3.490E+05 2.690 6450.0 C3H8+O=NC3H7+OH 3.710E+06 2.400 5505.0 C3H8+OH=NC3H7+H2O
1.050E+10 0.970 1586.0 C3H8+HO2=NC3H7+H2O2 4.080E+01 3.590 17160.0 C3H8+CH3=NC3H7+CH4
9.040E-01 3.650 7154.0 C3H8+C2H3=NC3H7+C2H4 1.000E+11 0.000 10400.0 C3H8+C2H5=NC3H7+C2H6
1.000E+11 0.000 10400.0 C3H8+C3H5-A=NC3H7+C3H6 7.940E+11 0.000 20500.0 C3H8+CH3O=NC3H7+CH3O
3.000E+11 0.000 7000.0 C3H8+CH3O2=NC3H7+CH3O2H 1.390E+00 3.970 18280.0 C3H8+C2H5O2=NC3H7+C
1.390E+00 3.970 18280.0 C3H8+NC3H7O2=NC3H7+NC3H7O2H 1.700E+13 0.000 20460.0 C3H8+IC3H7O2=NC
1.700E+13 0.000 20460.0 C3H8+CH3CO3=NC3H7+CH3CO3H 1.700E+13 0.000 20460.0 C3H8+O2CHO=NC3H7
5.520E+04 2.550 16480.0 IC3H7+H=C2H5+CH3 2.000E+13 0.000 0.0 IC3H7+OH=C3H6+H2O
2.410E+13 0.000 0.0 IC3H7+O=CH3COCH3+H 4.820E+13 0.000 0.0 IC3H7+O=CH3CHO+CH3
4.820E+13 0.000 0.0 NC3H7+HO2=NC3H7O+OH 7.000E+12 0.000 -1000.0 NC3H7+CH3O2=NC3H7O+CH3O
7.000E+12 0.000 -1000.0 IC3H7+HO2=IC3H7O+OH 7.000E+12 0.000 -1000.0 IC3H7+CH3O2=IC3H7O+CH3O
7.000E+12 0.000 -1000.0 C2H5+CH2O=NC3H7O 1.000E+11 0.000 3496.0 C2H5CHO+H=NC3H7O
4.000E+12 0.000 6260.0 CH3+CH3CHO=IC3H7O 1.000E+11 0.000 9256.0 CH3COCH3+H=IC3H7O
2.000E+12 0.000 7270.0 IC3H7O+O2=CH3COCH3+HO2 9.090E+09 0.000 390.0 NC3H7+O2=C3H6+HO2
1.310E-09 5.660 6061.0 DUP NC3H7+O2=C3H6+HO2 8.050E+00 3.320 12857.2 DUP NC3H7+O2=NC3H7O2
1.000E+11 0.000 0.0 PLOG / 1.00E-02 9.200E+08 0.405 -4399.0 / PLOG / 1.00E-01 1.450E+14
-0.984 -1711.0 / PLOG / 1.00E+00 2.090E+13 -0.499 -938.0 / PLOG / 1.00E+01 1.150E+20
-2.420 2451.0 / PLOG / 1.00E+02 2.070E+16 -1.300 803.0 / IC3H7+O2=IC3H7O2 1.000E+11
0.000 0.0 PLOG / 1.00E-02 7.330E+05 1.330 -6346.0 / PLOG / 1.00E-01 2.240E+11 -0.105 -
3698.0 / PLOG / 1.00E+00 1.540E+18 -2.020 -499.0 / PLOG / 1.00E+01 6.740E+27 -4.850
3780.0 / PLOG / 1.00E+02 1.670E+29 -5.150 5036.0 / IC3H7O2=C3H6+HO2 1.220E+09 1.280
30000.0 NC3H7O2=C3H6+HO2 6.240E+08 1.250 29600.0 NC3H7O2=C3H6OOH1-2 4.090E+08
1.100 30100.0 NC3H7O2=C3H6OOH1-3 3.570E+06 1.600 21000.0 IC3H7O2=C3H6OOH2-1 2.920E+09
1.100 33500.0 C3H6OOH1-2=C3H6O1-2+OH 1.210E+09 1.050 11300.0 C3H6OOH1-3=C3H6O1-
3+OH 2.640E+09 0.710 18500.0 C3H6OOH1-2=C3H6+HO2 2.340E+10 0.770 15300.0 C3H6OOH1-
3=¿OH+CH2O+C2H4 2.890E+09 1.300 26700.0 C3H6OOH2-1=C2H3OOH+CH3 8.560E+10 0.850
30700.0 C3H6OOH1-2=¿C2H4+CH2O+OH 1.310E+33 -7.010 48120.0 C3H6OOH1-2+O2=C3H6OOH1-
2O2 1.740E+14 -0.816 -536.0 C3H6OOH1-3+O2=C3H6OOH1-3O2 3.430E+16 -1.627 199.0 C3H6OOH2-

1+O2=C3H6OOH2-1O2 3.430E+16 -1.627 199.0 C3H6OOH1-2O2=C3H51-2,3OOH 2.920E+09
1.100 33500.0 C3H6OOH1-3O2=C3H52-1,3OOH 4.010E+08 1.100 30100.0 C3H6OOH2-1O2=C3H51-
2,3OOH 3.570E+06 1.600 21000.0 C3H51-2,3OOH=AC3H5OOH+HO2 2.560E+13 -0.490 17770.0
C3H52-1,3OOH=AC3H5OOH+HO2 1.150E+14 -0.630 17250.0 C3H51-2,3OOH=C3H5O1-2OOH-
3+OH 4.450E+09 0.860 10800.0 C3H51-2,3OOH=C3H5O1-3OOH-2+OH 2.640E+09 0.710 18500.0
C3H52-1,3OOH=C3H5O1-2OOH-3+OH 1.210E+09 1.050 11300.0 C3H5O1-2OOH-3=¿CH2CHO+CH2O+OH
1.000E+16 0.000 43000.0 C3H5O1-3OOH-2=¿CH2CHO+CH2O+OH 1.000E+16 0.000 43000.0
C3H6OOH1-2O2=C3KET12+OH 6.000E+11 0.000 26400.0 C3H6OOH1-3O2=C3KET13+OH 7.500E+10
0.000 21400.0 C3H6OOH2-1O2=C3KET21+OH 3.000E+11 0.000 23850.0 C3KET12=¿CH3CHO+HCO+OH
9.500E+15 0.000 42540.0 C3KET13=¿CH2O+CH2CHO+OH 1.000E+16 0.000 43000.0 C3KET21=¿CH2O+CH3C
1.000E+16 0.000 43000.0 C3KET21=¿OH+CH2O+CO+CH3 1.590E+20 -1.500 42879.0 C2H3OOH=CH2CHO+O
8.400E+14 0.000 43000.0 C2H3OOH=¿CH2CO+H+OH 1.590E+20 -1.500 42879.0 C3KET21=CH3COCH2O+OH
1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.490E+58 -13.900 54267.0 / PLOG / 1.00E-01 1.800E+54
-12.400 54194.0 / PLOG / 1.00E+00 3.360E+46 -9.810 52468.0 / PLOG / 1.00E+01 2.390E+36
-6.540 49429.0 / PLOG / 1.00E+02 1.280E+27 -3.610 46333.0 / NC3H7O2H=NC3H7O+OH
1.500E+16 0.000 42500.0 NC3H7O2+H2=NC3H7O2H+H 3.010E+13 0.000 26030.0 NC3H7O2+HO2=NC3H7O2H
1.750E+10 0.000 -3275.0 NC3H7O2+CH2O=NC3H7O2H+HCO 5.600E+12 0.000 13600.0 NC3H7O2+CH4=NC3H
1.120E+13 0.000 24640.0 NC3H7O2+CH3OH=NC3H7O2H+CH2OH 6.300E+12 0.000 19360.0
NC3H7O2+CH3CHO=NC3H7O2H+CH3CO 2.800E+12 0.000 13600.0 NC3H7O2+C2H4=NC3H7O2H+C2H3
1.130E+13 0.000 30430.0 NC3H7O2+C2H6=NC3H7O2H+C2H5 1.700E+13 0.000 20460.0 NC3H7O2+C2H3CHO=
2.800E+12 0.000 13600.0 NC3H7O2+C2H5CHO=NC3H7O2H+C2H5CO 2.000E+11 0.000 9500.0
NC3H7O2+NC3H7O2=¿NC3H7O+NC3H7O+O2 1.400E+16 -1.610 1860.0 NC3H7O2+CH3CO3=¿NC3H7O+CH3
1.400E+16 -1.610 1860.0 NC3H7O2+C2H5O2=¿NC3H7O+C2H5O+O2 1.400E+16 -1.610 1860.0
NC3H7O2+CH3=NC3H7O+CH3O 7.000E+12 0.000 -1000.0 NC3H7O2+C2H5=NC3H7O+C2H5O
7.000E+12 0.000 -1000.0 NC3H7O2+IC3H7=NC3H7O+IC3H7O 7.000E+12 0.000 -1000.0 NC3H7O2+NC3H7=NC
7.000E+12 0.000 -1000.0 NC3H7O2+C3H5-A=NC3H7O+C3H5O 7.000E+12 0.000 -1000.0 NC3H7O2+CH3O2=¿
1.400E+16 -1.610 1860.0 IC3H7O+OH=IC3H7O2H 1.000E+15 -0.800 0.0 IC3H7O2+H2=IC3H7O2H+H
3.010E+13 0.000 26030.0 IC3H7O2+HO2=IC3H7O2H+O2 1.750E+10 0.000 -3275.0 IC3H7O2+CH2O=IC3H7O2H
5.600E+12 0.000 13600.0 IC3H7O2+CH4=IC3H7O2H+CH3 1.120E+13 0.000 24640.0 IC3H7O2+CH3CHO=IC3H7
2.800E+12 0.000 13600.0 IC3H7O2+C2H4=IC3H7O2H+C2H3 1.130E+13 0.000 30430.0 IC3H7O2+CH3OH=IC3H
6.300E+12 0.000 19360.0 IC3H7O2+C2H6=IC3H7O2H+C2H5 1.700E+13 0.000 20460.0 IC3H7O2+C2H3CHO=IC
2.800E+12 0.000 13600.0 IC3H7O2+C2H5CHO=IC3H7O2H+C2H5CO 2.000E+11 0.000 9500.0
IC3H7O2+CH3O2=¿IC3H7O+CH3O+O2 1.400E+16 -1.610 1860.0 IC3H7O2+CH3CO3=¿IC3H7O+CH3CO2+O2
1.400E+16 -1.610 1860.0 IC3H7O2+C2H5O2=¿IC3H7O+C2H5O+O2 1.400E+16 -1.610 1860.0
IC3H7O2+IC3H7O2=¿O2+IC3H7O+IC3H7O 1.400E+16 -1.610 1860.0 IC3H7O2+NC3H7O2=¿IC3H7O+NC3H7O
1.400E+16 -1.610 1860.0 IC3H7O2+CH3=IC3H7O+CH3O 7.000E+12 0.000 -1000.0 IC3H7O2+C2H5=IC3H7O+C

7.000E+12 0.000 -1000.0 IC3H7O2+IC3H7=IC3H7O+IC3H7O 7.000E+12 0.000 -1000.0 IC3H7O2+NC3H7=IC3H7
7.000E+12 0.000 -1000.0 IC3H7O2+C3H5-A=IC3H7O+C3H5O 7.000E+12 0.000 -1000.0 C3H6O1-
2=C2H4+CH2O 6.000E+14 0.000 60000.0 C3H6O1-2+OH=¿CH2O+C2H3+H2O 5.000E+12 0.000
0.0 C3H6O1-2+H=¿CH2O+C2H3+H2 2.630E+07 2.000 5000.0 C3H6O1-2+O=¿CH2O+C2H3+OH
8.430E+13 0.000 5200.0 C3H6O1-2+HO2=¿CH2O+C2H3+H2O2 1.000E+13 0.000 15000.0 C3H6O1-
2+CH3O2=¿CH2O+C2H3+CH3O2H 1.000E+13 0.000 19000.0 C3H6O1-2+CH3=¿CH2O+C2H3+CH4
2.000E+11 0.000 10000.0 C3H6O1-3=C2H4+CH2O 6.000E+14 0.000 60000.0 C3H6O1-3+OH=¿CH2O+C2H3+H2
5.000E+12 0.000 0.0 C3H6O1-3+O=¿CH2O+C2H3+OH 8.430E+13 0.000 5200.0 C3H6O1-3+H=¿CH2O+C2H3+
2.630E+07 2.000 5000.0 C3H6O1-3+CH3O2=¿CH2O+C2H3+CH3O2H 1.000E+13 0.000 19000.0
C3H6O1-3+HO2=¿CH2O+C2H3+H2O2 1.000E+13 0.000 15000.0 C3H6O1-3+CH3=¿CH2O+C2H3+CH4
2.000E+11 0.000 10000.0 C2H3+CH3(+M)=C3H6(+M) 2.500E+13 0.000 0.0 LOW / 4.270E+58
-11.940 9770.0 / TROE / 1.750E-01 1.341E+03 6.000E+04 1.014E+04 / CH2(S)+C2H4=CC3H6
1.440E+51 -13.100 14200.0 PLOG / 1.00E-02 1.440E+51 -13.100 14200.0 / PLOG / 1.00E-01
3.380E+54 -13.600 16500.0 / PLOG / 1.00E+00 1.350E+54 -13.000 18900.0 / PLOG / 1.00E+01
2.730E+47 -10.800 14200.0 / PLOG / 1.00E+02 2.710E+50 -11.200 16700.0 / DUP CH2(S)+C2H4=CC3H6
6.160E+40 -10.500 5428.0 PLOG / 1.00E-02 6.160E+40 -10.500 5428.0 / PLOG / 1.00E-01
6.930E+41 -10.300 6189.0 / PLOG / 1.00E+00 1.810E+37 -8.550 5521.0 / PLOG / 1.00E+01
4.260E+37 -8.320 4770.0 / PLOG / 1.00E+02 4.680E+35 -7.370 4689.0 / DUP CH2(S)+C2H4=C3H6
4.820E+57 -14.300 17100.0 PLOG / 1.00E-02 4.820E+57 -14.300 17100.0 / PLOG / 1.00E-01
3.840E+59 -14.400 18400.0 / PLOG / 1.00E+00 2.130E+58 -13.500 20400.0 / PLOG / 1.00E+01
8.480E+52 -11.600 20700.0 / PLOG / 1.00E+02 6.070E+47 -9.850 22100.0 / DUP CH2(S)+C2H4=C3H6
1.150E+45 -11.100 6145.0 PLOG / 1.00E-02 1.150E+45 -11.100 6145.0 / PLOG / 1.00E-01
1.830E+45 -10.700 6638.0 / PLOG / 1.00E+00 1.300E+40 -8.770 5864.0 / PLOG / 1.00E+01
2.270E+32 -6.140 4318.0 / PLOG / 1.00E+02 1.280E+24 -3.490 2530.0 / DUP CH2(S)+C2H4=C3H5-
A+H 8.200E+19 -2.060 1150.0 PLOG / 1.00E-02 8.200E+19 -2.060 1150.0 / PLOG / 1.00E-01
2.270E+21 -2.440 2650.0 / PLOG / 1.00E+00 4.440E+35 -6.550 13900.0 / PLOG / 1.00E+01
1.180E+28 -4.090 14000.0 / PLOG / 1.00E+02 6.510E+26 -3.580 18900.0 / DUP CH2(S)+C2H4=C3H5-
A+H 1.080E+07 1.620 -3175.0 PLOG / 1.00E-02 1.080E+07 1.620 -3175.0 / PLOG / 1.00E-01
1.370E+05 2.150 -3799.0 / PLOG / 1.00E+00 3.890E+14 -0.420 1238.0 / PLOG / 1.00E+01
2.450E+10 0.670 751.0 / PLOG / 1.00E+02 1.810E+02 2.970 -746.0 / DUP CH2(S)+C2H4=C2H3+CH3
1.770E+19 -1.940 6790.0 PLOG / 1.00E-02 1.770E+19 -1.940 6790.0 / PLOG / 1.00E-01 1.680E+19
-1.800 4310.0 / PLOG / 1.00E+00 4.160E+24 -3.190 9760.0 / PLOG / 1.00E+01 7.890E+24 -
3.070 13900.0 / PLOG / 1.00E+02 7.360E+29 -4.280 23800.0 / DUP CH2(S)+C2H4=C2H3+CH3
4.300E+12 0.190 -110.0 PLOG / 1.00E-02 4.300E+12 0.190 -110.0 / PLOG / 1.00E-01 2.260E+11
0.540 48.0 / PLOG / 1.00E+00 4.920E+09 1.020 600.0 / PLOG / 1.00E+01 1.470E+08 1.330
1228.0 / PLOG / 1.00E+02 8.110E+10 0.550 5506.0 / DUP C2H3+CH3=C3H5-A+H 4.120E+29

-4.950 8000.0 PLOG / 1.00E-02 4.120E+29 -4.950 8000.0 / PLOG / 1.00E-01 4.860E+30 -5.030 11300.0 / PLOG / 1.00E+00 5.300E+29 -4.570 14400.0 / PLOG / 1.00E+01 1.320E+30 -4.540 19300.0 / PLOG / 1.00E+02 5.160E+28 -4.030 23800.0 / DUP C2H3+CH3=C3H5-A+H 5.730E+15 -0.770 1196.0 PLOG / 1.00E-02 5.730E+15 -0.770 1196.0 / PLOG / 1.00E-01 2.060E+13 -0.074 1429.0 / PLOG / 1.00E+00 4.480E+10 0.600 1422.0 / PLOG / 1.00E+01 4.100E+06 1.710 1057.0 / PLOG / 1.00E+02 1.370E-01 3.910 -354.0 / DUP C3H6=C2H3+CH3 1.880E+78 -18.700 130000.0 PLOG / 1.00E-02 1.880E+78 -18.700 130000.0 / PLOG / 1.00E-01 8.730E+76 -17.900 132000.0 / PLOG / 1.00E+00 5.800E+75 -17.200 134000.0 / PLOG / 1.00E+01 8.120E+71 -15.800 136000.0 / PLOG / 1.00E+02 2.150E+64 -13.400 135000.0 / DUP C3H6=C2H3+CH3 1.690E+59 -13.600 113290.0 PLOG / 1.00E-02 1.690E+59 -13.600 113290.0 / PLOG / 1.00E-01 2.000E+60 -13.700 114890.0 / PLOG / 1.00E+00 6.700E+54 -11.800 113840.0 / PLOG / 1.00E+01 1.060E+47 -9.270 111510.0 / PLOG / 1.00E+02 7.290E+38 -6.700 108740.0 / DUP C3H6=C3H5-A+H 9.160E+74 -17.600 120000.0 PLOG / 1.00E-02 9.160E+74 -17.600 120000.0 / PLOG / 1.00E-01 1.730E+70 -16.000 120000.0 / PLOG / 1.00E+00 1.080E+71 -15.900 124860.0 / PLOG / 1.00E+01 6.400E+65 -14.200 125000.0 / PLOG / 1.00E+02 8.050E+56 -11.500 122000.0 / DUP C3H6=C3H5-A+H 2.980E+54 -12.300 101200.0 PLOG / 1.00E-02 2.980E+54 -12.300 101200.0 / PLOG / 1.00E-01 1.370E+43 -8.870 96365.0 / PLOG / 1.00E+00 6.280E+42 -8.510 98004.0 / PLOG / 1.00E+01 4.730E+35 -6.260 95644.0 / PLOG / 1.00E+02 4.340E+28 -4.060 93114.0 / DUP C3H6=CC3H6 1.260E+64 -15.600 95000.0 PLOG / 1.00E-02 1.260E+64 -15.600 95000.0 / PLOG / 1.00E-01 3.940E+67 -16.200 101000.0 / PLOG / 1.00E+00 6.140E+68 -16.200 106000.0 / PLOG / 1.00E+01 9.700E+66 -15.300 109000.0 / PLOG / 1.00E+02 1.450E+62 -13.600 110000.0 / DUP C3H6=CC3H6 4.840E+41 -9.620 79528.0 PLOG / 1.00E-02 4.840E+41 -9.620 79528.0 / PLOG / 1.00E-01 8.070E+44 -10.200 82671.0 / PLOG / 1.00E+00 1.150E+47 -10.600 85502.0 / PLOG / 1.00E+01 1.330E+39 -7.980 83303.0 / PLOG / 1.00E+02 4.970E+31 -5.600 80987.0 / DUP CC3H6=C3H5-A+H 2.330E+63 -14.600 103000.0 PLOG / 1.00E-02 2.330E+63 -14.600 103000.0 / PLOG / 1.00E-01 7.030E+63 -14.400 107000.0 / PLOG / 1.00E+00 5.070E+64 -14.300 112000.0 / PLOG / 1.00E+01 4.920E+61 -13.200 115000.0 / PLOG / 1.00E+02 4.820E+57 -11.700 118000.0 / DUP CC3H6=C3H5-A+H 1.120E+40 -8.370 85836.0 PLOG / 1.00E-02 1.120E+40 -8.370 85836.0 / PLOG / 1.00E-01 1.060E+41 -8.330 88499.0 / PLOG / 1.00E+00 8.230E+43 -8.880 92907.0 / PLOG / 1.00E+01 1.270E+39 -7.330 93401.0 / PLOG / 1.00E+02 1.450E+28 -4.020 90995.0 / DUP CC3H6=C2H3+CH3 8.310E+64 -15.100 111000.0 PLOG / 1.00E-02 8.310E+64 -15.100 111000.0 / PLOG / 1.00E-01 8.290E+64 -14.700 114000.0 / PLOG / 1.00E+00 1.000E+70 -15.700 122000.0 / PLOG / 1.00E+01 1.660E+67 -14.600 124000.0 / PLOG / 1.00E+02 7.870E+62 -13.100 127000.0 / DUP CC3H6=C2H3+CH3 1.510E+49 -11.000 99748.0 PLOG / 1.00E-02 1.510E+49 -11.000 99748.0 / PLOG / 1.00E-01 1.050E+45 -9.460 99275.0 / PLOG / 1.00E+00 3.390E+50 -10.600 104220.0 / PLOG / 1.00E+01 1.760E+47 -9.430 104930.0 / PLOG / 1.00E+02 1.880E+39 -

6.930 103980.0 / DUP C3H5-T+H=C3H6 4.960E+60 -15.200 18000.0 PLOG / 1.00E-02 4.960E+60 -15.200 18000.0 / PLOG / 1.00E-01 3.200E+62 -15.100 20100.0 / PLOG / 1.00E+00 2.310E+60 -14.000 21900.0 / PLOG / 1.00E+01 3.690E+54 -12.000 22100.0 / PLOG / 1.00E+02 1.150E+50 -10.400 23300.0 / DUP C3H5-T+H=C3H6 1.490E+48 -12.000 7203.0 PLOG / 1.00E-02 1.490E+48 -12.000 7203.0 / PLOG / 1.00E-01 6.760E+46 -11.100 7630.0 / PLOG / 1.00E+00 1.090E+40 -8.660 6448.0 / PLOG / 1.00E+01 2.380E+31 -5.730 4506.0 / PLOG / 1.00E+02 5.690E+25 -3.830 3250.0 / DUP C3H5-T+H=C3H5-A+H 2.110E+17 -1.080 1290.0 PLOG / 1.00E-02 2.110E+17 -1.080 1290.0 / PLOG / 1.00E-01 9.050E+29 -4.910 8540.0 / PLOG / 1.00E+00 2.980E+30 -4.790 12000.0 / PLOG / 1.00E+01 8.220E+28 -4.140 15400.0 / PLOG / 1.00E+02 2.280E+29 -4.120 20900.0 / DUP C3H5-T+H=C3H5-A+H 6.410E+03 2.610 -3778.0 PLOG / 1.00E-02 6.410E+03 2.610 -3778.0 / PLOG / 1.00E-01 5.190E+14 -0.300 1090.0 / PLOG / 1.00E+00 8.170E+11 0.490 1185.0 / PLOG / 1.00E+01 2.790E+09 1.090 1188.0 / PLOG / 1.00E+02 6.750E+03 2.700 374.0 / DUP C3H5-T+H=C2H3+CH3 3.310E+16 -0.690 5200.0 PLOG / 1.00E-02 3.310E+16 -0.690 5200.0 / PLOG / 1.00E-01 9.040E+16 -0.810 4800.0 / PLOG / 1.00E+00 2.010E+24 -2.860 10900.0 / PLOG / 1.00E+01 2.750E+26 -3.310 15800.0 / PLOG / 1.00E+02 3.150E+32 -4.830 26000.0 / DUP C3H5-T+H=C2H3+CH3 8.040E+13 -0.140 1150.0 PLOG / 1.00E-02 8.040E+13 -0.140 1150.0 / PLOG / 1.00E-01 7.170E+10 0.670 674.0 / PLOG / 1.00E+00 9.970E+08 1.360 1596.0 / PLOG / 1.00E+01 7.410E+07 1.570 2109.0 / PLOG / 1.00E+02 2.700E+12 0.320 6792.0 / DUP C3H6=C3H5-S+H 7.710E+69 -16.090 140000.0 C3H6+H=C3H5-A+H2 3.640E+05 2.455 4361.0 C3H6+O2=C3H5-A+HO2 5.960E+19 -1.670 46192.0 C3H6+O=C3H5-A+OH 5.240E+11 0.700 5884.0 C3H6+OH=C3H5-A+H2O 4.460E+06 2.072 1051.0 C3H6+HO2=C3H5-A+H2O2 3.070E-02 4.403 13547.0 C3H6+CH3=C3H5-A+CH4 2.210E+00 3.500 5675.0 C3H6+CH3O=C3H5-A+CH3OH 8.400E+10 0.000 2600.0 C3H6+CH3O2=C3H5-A+CH3O2H 7.680E-02 4.403 13547.0 C3H6+C2H5=C3H5-A+C2H6 1.000E+11 0.000 9800.0 C3H6+C2H5O2=C3H5-A+C2H5O2H 7.680E-02 4.403 13547.0 C3H6+CH3CO3=C3H5-A+CH3CO3H 7.680E-02 4.403 13547.0 C3H6+NC3H7O2=C3H5-A+NC3H7O2H 7.680E-02 4.403 13547.0 C3H6+IC3H7O2=C3H5-A+IC3H7O2H 7.680E-02 4.403 13547.0

C3H6+H=C3H5-T+H2 1.500E+02 3.381 8910.0 C3H6+O=C3H5-T+OH 6.030E+10 0.700 7632.0 C3H6+OH=C3H5-T+H2O 1.800E+06 1.979 2235.0 C3H6+HO2=C3H5-T+H2O2 1.560E+04 2.820 24428.0 C3H6+O2=C3H5-T+HO2 1.000E+13 0.000 58770.0 C3H6+CH3=C3H5-T+CH4 8.400E-01 3.500 11660.0

C3H6+H=C3H5-S+H2 5.100E+02 3.234 12357.0 DUP C3H6+H=C3H5-S+H2 3.970E+02 3.252 12007.0 DUP C3H6+O2=C3H5-S+HO2 2.000E+13 0.000 62270.0 C3H6+O=C3H5-S+OH 1.200E+11 0.700 8959.0 C3H6+OH=C3H5-S+H2O 1.860E+05 2.369 2502.0 C3H6+HO2=C3H5-S+H2O2 9.570E+02 3.059 20799.0 C3H6+CH3=C3H5-S+CH4 1.350E+00 3.500 12850.0 C3H6+O=C2H5+HCO 7.450E+06 1.880 183.0 C3H6+O=¿CH2CO+CH3+H 3.050E+06 1.880 183.0 C3H6+O=¿CH3CHCO+H+H

3.050E+06 1.880 183.0 C3H6+H=NC3H7 1.000E+00 1.000 0.0 PLOG / 1.30E-03 7.990E+81 -23.161 22239.0 / PLOG / 4.00E-02 4.240E+68 -18.427 19665.0 / PLOG / 1.00E+00 1.040E+49 -11.500 15359.0 / PLOG / 1.00E+01 6.200E+41 -8.892 14637.0 / PLOG / 1.00E+02 1.000E-10 0.000 0.0 / DUP C3H6+H=NC3H7 1.000E+00 1.000 0.0 PLOG / 1.30E-03 1.850E+26 -5.830 3866.0 / PLOG / 4.00E-02 2.820E+30 -6.490 5471.0 / PLOG / 1.00E+00 3.780E+28 -5.570 5625.0 / PLOG / 1.00E+01 1.460E+25 -4.280 5248.0 / PLOG / 1.00E+02 4.220E+27 -4.390 9346.0 / DUP C3H6+H=C2H4+CH3 1.000E+00 1.000 1.0 PLOG / 1.30E-03 1.540E+09 1.350 2542.0 / PLOG / 4.00E-02 7.880E+10 0.870 3600.0 / PLOG / 1.00E+00 2.670E+12 0.470 5431.0 / PLOG / 1.00E+01 9.250E+22 -2.600 12898.0 / PLOG / 1.00E+02 1.320E+23 -2.420 16500.0 / DUP C3H6+H=C2H4+CH3 1.000E+00 1.000 1.0 PLOG / 1.30E-03 1.000E-10 0.000 0.0 / PLOG / 4.00E-02 1.000E-10 0.000 0.0 / PLOG / 1.00E+00 1.000E-10 0.000 0.0 / PLOG / 1.00E+01 1.240E+05 2.520 3679.0 / PLOG / 1.00E+02 2.510E+03 2.910 3981.0 / DUP C3H6+H=IC3H7 1.000E+00 1.000 1.0 PLOG / 1.30E-03 1.350E+44 -10.680 8196.0 / PLOG / 4.00E-02 2.110E+57 -14.230 15147.0 / PLOG / 1.00E+00 3.260E+61 -14.940 20161.0 / PLOG / 1.00E+01 5.300E+56 -13.120 20667.0 / PLOG / 1.00E+02 1.110E+50 -10.800 20202.0 / DUP C3H6+H=IC3H7 1.000E+00 1.000 1.0 PLOG / 1.30E-03 2.170E+130 -32.580 136140.0 / PLOG / 4.00E-02 2.250E+29 -5.840 4242.0 / PLOG / 1.00E+00 1.060E+30 -5.630 5613.0 / PLOG / 1.00E+01 6.110E+26 -4.440 5182.0 / PLOG / 1.00E+02 2.730E+23 -3.260 4597.0 / DUP C2H4+CH3=NC3H7 1.000E+00 1.000 1.0 PLOG / 1.30E-03 8.670E+48 -12.540 18206.0 / PLOG / 4.00E-02 1.060E+49 -12.040 20001.0 / PLOG / 1.00E+00 7.670E+47 -11.170 22366.0 / PLOG / 1.00E+01 1.810E+45 -10.030 23769.0 / PLOG / 1.00E+02 2.040E+40 -8.250 24214.0 / DUP C2H4+CH3=NC3H7 1.000E+00 1.000 1.0 PLOG / 1.30E-03 1.120E+43 -11.300 13080.0 / PLOG / 4.00E-02 7.280E+39 -9.880 13164.0 / PLOG / 1.00E+00 2.600E+33 -7.460 12416.0 / PLOG / 1.00E+01 3.850E+27 -5.380 11455.0 / PLOG / 1.00E+02 1.660E+21 -3.170 10241.0 / DUP C3H6+HO2=C3H6OOH2-1 4.850E-21 2.650 11201.0 PLOG / 1.30E-02 1.310E+13 -1.840 8561.0 / PLOG / 9.87E-01 5.930E+17 -2.610 11533.0 / PLOG / 9.87E+00 8.340E+24 -4.400 16440.0 / PLOG / 9.87E+01 3.750E+23 -3.680 17965.0 / C3H6+HO2=C3H6O1-2+OH 1.130E+19 -1.680 23587.0 PLOG / 1.30E-02 3.730E+03 2.640 11173.0 / PLOG / 9.87E-01 1.780E+12 0.110 16137.0 / PLOG / 9.87E+00 3.900E+17 -1.400 20077.0 / PLOG / 9.87E+01 1.130E+19 -1.680 23587.0 / C3H6+HO2=IC3H7+O2 8.870E+22 -3.090 26586.0 PLOG / 1.30E-02 1.020E+07 1.160 10273.0 / PLOG / 9.87E-01 1.310E+20 -2.580 19078.0 / PLOG / 9.87E+00 4.140E+28 -4.920 26212.0 / PLOG / 9.87E+01 8.870E+22 -3.090 26586.0 / C3H6OOH2-1=C3H6O1-2+OH 6.910E+07 1.370 13373.0 PLOG / 1.30E-02 2.660E+35 -8.360 18056.0 / PLOG / 9.87E-01 1.960E+35 -7.660 20595.0 / PLOG / 9.87E+00 2.240E+33 -6.750 21619.0 / PLOG / 9.87E+01 8.480E+26 -4.580 20278.0 / C3H5-A+H=C3H4-A+H2 1.230E+03 3.035 2582.0 C3H5-A+OH=C3H4-A+H2O 6.000E+12 0.000 0.0 C3H5-A+CH3=C3H4-A+CH4 3.000E+12 -0.320 -131.0 C3H5-A+C2H5=C3H4-A+C2H6 4.000E+11 0.000 0.0 C3H5-A+C2H3=C3H4-

A+C2H4 1.000E+12 0.000 0.0 C3H4-A+C3H4-A=C3H5-A+C3H3 5.000E+14 0.000 64747.0 C3H5-S+H=C3H4-A+H2 3.330E+12 0.000 0.0 C3H5-S+CH3=C3H4-A+CH4 1.000E+11 0.000 0.0 C3H5-S+H=C3H4-P+H2 3.340E+12 0.000 0.0 C3H5-S+CH3=C3H4-P+CH4 1.000E+11 0.000 0.0

C3H5-T+H=C3H4-P+H2 3.340E+12 0.000 0.0 C3H5-T+CH3=C3H4-P+CH4 1.000E+11 0.000 0.0 C3H5-A+C3H5-A=C3H4-A+C3H6 9.550E+40 -9.300 12470.0 PLOG / 1.00E+00 4.770E+40 -9.300 12470.0 / PLOG / 4.00E+00 3.970E+32 -6.800 9180.0 / PLOG / 1.00E+01 1.460E+28 -5.500 7410.0 / C3H5-A+C2H5=C2H4+C3H6 4.000E+11 0.000 0.0 C3H5-A+HCO=C3H6+CO 6.000E+13 0.000 0.0 C3H5-S+HCO=C3H6+CO 9.000E+13 0.000 0.0 C3H5-T+HCO=C3H6+CO 9.000E+13 0.000 0.0 C3H5-S+O=C2H4+HCO 6.000E+13 0.000 0.0 C3H5-S+OH=¿C2H4+HCO+H 5.000E+12 0.000 0.0 C3H5-S+HO2=¿C2H4+HCO+OH 2.000E+13 0.000 0.0

C3H5-T+O=CH3+CH2CO 6.000E+13 0.000 0.0 C3H5-T+OH=¿CH3+CH2CO+H 5.000E+12 0.000 0.0 C3H5-T+HO2=¿CH3+CH2CO+OH 2.000E+13 0.000 0.0 C3H5-A+O=C2H3CHO+H 6.000E+13 0.000 0.0 C3H5-A+OH=¿C2H3CHO+H+H 5.300E+37 -6.710 29306.0 PLOG / 1.00E-01 5.300E+37 -6.710 29306.0 / PLOG / 1.00E+00 4.200E+32 -5.160 30126.0 / PLOG / 1.00E+01 1.600E+20 -1.560 26330.0 / C3H5-A+O2=C3H4-A+HO2 4.990E+15 -1.400 22428.0 PLOG / 1.00E+00 4.990E+15 -1.400 22428.0 / PLOG / 1.00E+01 2.180E+21 -2.850 30755.0 / C3H5-A+O2=CH3CO+CH2O 1.190E+15 -1.010 20128.0 PLOG / 1.00E+00 1.190E+15 -1.010 20128.0 / PLOG / 1.00E+01 7.140E+15 -1.210 21046.0 / C3H5-A+O2=C2H3CHO+OH 1.820E+13 -0.410 22859.0 PLOG / 1.00E+00 1.820E+13 -0.410 22859.0 / PLOG / 1.00E+01 2.470E+13 -0.450 23017.0 / C3H5-S+O2=CH3CHO+HCO 3.100E+31 -5.944 5748.0 C3H5-S+O2=CH3CHCHO+O 5.380E+18 -2.140 5143.0 C3H5-S+O2=C2H3CHO+OH 2.700E+19 -2.140 5143.0 C3H5-T+O2=CH3COCH2+O 9.860E+25 -3.751 11255.0 C3H5-T+O2=CH3CO+CH2O 2.550E+20 -2.608 1566.0 C3H5-T+O2=C3H4-A+HO2 3.590E+10 -0.270 -414.0 C3H5-A+HO2=C3H5O+OH 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.020E+13 -0.158 -1417.0 / PLOG / 1.00E-01 4.980E+14 -0.642 -349.0 / PLOG / 1.00E+00 7.770E+17 -1.520 2379.0 / PLOG / 1.00E+01 2.930E+15 -0.684 3615.0 / PLOG / 1.00E+02 1.640E+04 2.740 1144.0 / C3H5-A+HO2=AC3H5OOH 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.910E+31 -7.230 1336.0 / PLOG / 1.00E-01 6.310E+42 -10.300 5569.0 / PLOG / 1.00E+00 1.030E+45 -10.600 7852.0 / PLOG / 1.00E+01 2.790E+37 -7.920 6498.0 / PLOG / 1.00E+02 1.440E+32 -6.010 6054.0 / C3H5-A+HO2=C2H3CHO+H2O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.090E+00 3.010 -3421.0 / PLOG / 1.00E-01 6.350E+01 2.500 -2341.0 / PLOG / 1.00E+00 6.050E+05 1.390 595.0 / PLOG / 1.00E+01 3.100E+05 1.590 2678.0 / PLOG / 1.00E+02 5.070E-05 4.590 928.0 / AC3H5OOH=C2H3CHO+H2O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.990E+50 -12.700 53532.0 / PLOG / 1.00E-01 4.720E+47 -11.500 54361.0 / PLOG / 1.00E+00 1.500E+40 -8.840 53179.0 / PLOG / 1.00E+01 2.540E+28 -5.000 49919.0 / PLOG / 1.00E+02 1.480E+16 -1.120 45949.0 / AC3H5OOH=C3H5O+OH 1.000E+11 0.000 0.0 PLOG

/ 1.00E-02 1.490E+58 -13.900 54267.0 / PLOG / 1.00E-01 1.800E+54 -12.400 54194.0 / PLOG / 1.00E+00 3.360E+46 -9.810 52468.0 / PLOG / 1.00E+01 2.390E+36 -6.540 49429.0 / PLOG / 1.00E+02 1.280E+27 -3.610 46333.0 / C3H5O=C2H3+CH2O 1.000E+11 0.000 0.0 PLOG / 1.00E-03 7.260E+06 0.182 17816.0 / PLOG / 1.00E-02 6.970E+16 -2.500 20879.0 / PLOG / 1.00E-01 6.640E+23 -4.230 23565.0 / PLOG / 1.00E+00 1.070E+26 -4.560 24623.0 / PLOG / 1.00E+01 6.500E+29 -5.370 26645.0 / PLOG / 1.00E+02 4.630E+31 -5.590 28915.0 / PLOG / 1.00E+03 8.520E+25 -3.610 27863.0 / C3H5O=CH2CHOCH2 1.000E+11 0.000 0.0 PLOG / 1.00E-03 3.170E+20 -4.150 12121.0 / PLOG / 1.00E-02 4.790E+24 -5.030 14606.0 / PLOG / 1.00E-01 1.900E+26 -5.160 16124.0 / PLOG / 1.00E+00 1.510E+28 -5.400 18165.0 / PLOG / 1.00E+01 2.420E+28 -5.170 19691.0 / PLOG / 1.00E+02 5.570E+24 -3.860 19395.0 / PLOG / 1.00E+03 1.350E+18 -1.730 17386.0 / C3H5O=CH2CH2CHO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 5.250E-49 15.500 -15640.0 / PLOG / 1.00E-02 1.460E-88 27.600 -35995.0 / PLOG / 1.00E-01 4.440E-22 8.380 -3819.0 / PLOG / 1.00E+00 6.230E+12 -1.440 10829.0 / PLOG / 1.00E+01 3.480E+42 -9.910 25298.0 / PLOG / 1.00E+02 1.880E+38 -8.160 25974.0 / PLOG / 1.00E+03 1.670E+21 -2.740 20338.0 / C3H5O=C2H3CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 3.000E+15 -2.310 14668.0 / PLOG / 1.00E-02 1.500E+22 -3.960 18283.0 / PLOG / 1.00E-01 1.950E+23 -3.990 19143.0 / PLOG / 1.00E+00 1.150E+25 -4.240 20311.0 / PLOG / 1.00E+01 1.760E+28 -4.890 22765.0 / PLOG / 1.00E+02 1.410E+27 -4.280 23771.0 / PLOG / 1.00E+03 2.570E+20 -2.060 22040.0 / C3H5O=C2H4+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 6.620E+16 -2.840 13197.0 / PLOG / 1.00E-02 1.260E+20 -3.530 15469.0 / PLOG / 1.00E-01 2.130E+21 -3.640 16584.0 / PLOG / 1.00E+00 1.070E+24 -4.160 18985.0 / PLOG / 1.00E+01 8.420E+25 -4.400 22383.0 / PLOG / 1.00E+02 1.860E+21 -2.730 23659.0 / PLOG / 1.00E+03 4.750E+08 1.140 20922.0 / CH2CHOCH2=C2H3+CH2O 1.000E+11 0.000 0.0 PLOG / 1.00E-03 3.300E+09 -0.638 19748.0 / PLOG / 1.00E-02 3.360E+21 -3.900 23945.0 / PLOG / 1.00E-01 2.910E+29 -5.900 27250.0 / PLOG / 1.00E+00 1.830E+34 -6.940 30690.0 / PLOG / 1.00E+01 9.720E+33 -6.500 33002.0 / PLOG / 1.00E+02 2.680E+27 -4.260 33306.0 / PLOG / 1.00E+03 8.810E+14 -0.326 31553.0 / CH2CHOCH2=CH2CH2CHO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 8.010E-92 27.800 -37321.0 / PLOG / 1.00E-02 7.780E-11 3.700 -2767.0 / PLOG / 1.00E-01 5.110E+15 -2.760 15938.0 / PLOG / 1.00E+00 4.480E+25 -5.200 21532.0 / PLOG / 1.00E+01 3.970E+34 -7.410 28117.0 / PLOG / 1.00E+02 5.620E+22 -3.560 25807.0 / PLOG / 1.00E+03 2.510E+20 -2.630 29288.0 / CH2CHOCH2=C2H3CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 4.930E+24 -5.050 20108.0 / PLOG / 1.00E-02 2.140E+28 -5.800 22219.0 / PLOG / 1.00E-01 1.930E+32 -6.640 25108.0 / PLOG / 1.00E+00 8.600E+34 -7.110 28209.0 / PLOG / 1.00E+01 2.170E+34 -6.640 30648.0 / PLOG / 1.00E+02 4.170E+28 -4.710 31232.0 / PLOG / 1.00E+03 3.980E+18 -1.620 30130.0 / CH2CHOCH2=C2H4+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 8.230E+26 -5.840 19357.0 / PLOG / 1.00E-02 1.320E+29 -6.210 21294.0 / PLOG / 1.00E-01 3.470E+32

-6.960 24197.0 / PLOG / 1.00E+00 1.440E+36 -7.760 28008.0 / PLOG / 1.00E+01 9.720E+37 -8.020 32395.0 / PLOG / 1.00E+02 2.430E+31 -5.810 34296.0 / PLOG / 1.00E+03 3.730E+14 -0.726 32008.0 / CH2CH2CHO=C2H3+CH2O 1.000E+11 0.000 0.0 PLOG / 1.00E-03 6.890E-69 21.500 2638.0 / PLOG / 1.00E-02 5.340E-33 11.100 16749.0 / PLOG / 1.00E-01 6.110E+26 -6.010 44117.0 / PLOG / 1.00E+00 8.040E+35 -8.310 46920.0 / PLOG / 1.00E+01 5.520E+40 -9.190 50509.0 / PLOG / 1.00E+02 5.850E+35 -7.180 52038.0 / PLOG / 1.00E+03 1.930E+19 -1.940 48440.0 / CH2CH2CHO=C2H3CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 1.610E+10 -1.240 32371.0 / PLOG / 1.00E-02 5.840E+15 -2.610 32878.0 / PLOG / 1.00E-01 3.640E+23 -4.600 34275.0 / PLOG / 1.00E+00 7.580E+31 -6.630 37895.0 / PLOG / 1.00E+01 2.860E+32 -6.300 39991.0 / PLOG / 1.00E+02 1.570E+23 -3.140 38012.0 / PLOG / 1.00E+03 4.520E+12 0.214 34570.0 / CH2CH2CHO=C2H4+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 2.900E+32 -7.240 25688.0 / PLOG / 1.00E-02 5.300E+33 -7.280 27101.0 / PLOG / 1.00E-01 2.000E+35 -7.410 29027.0 / PLOG / 1.00E+00 1.010E+34 -6.700 30018.0 / PLOG / 1.00E+01 9.760E+27 -4.630 28924.0 / PLOG / 1.00E+02 2.110E+19 -1.850 26240.0 / PLOG / 1.00E+03 1.590E+13 0.063 24086.0 / C2H3+CH2O=C2H3CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 2.600E+04 2.260 1510.0 / PLOG / 1.00E-02 5.130E+04 2.170 1676.0 / PLOG / 1.00E-01 3.990E+05 1.910 2218.0 / PLOG / 1.00E+00 1.750E+07 1.450 3428.0 / PLOG / 1.00E+01 1.350E+09 0.933 5173.0 / PLOG / 1.00E+02 2.240E+11 0.357 8001.0 / PLOG / 1.00E+03 6.010E+05 2.090 7896.0 / C2H3+CH2O=C2H4+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 1.110E+07 1.090 1807.0 / PLOG / 1.00E-02 2.470E+07 0.993 1995.0 / PLOG / 1.00E-01 2.470E+08 0.704 2596.0 / PLOG / 1.00E+00 1.420E+10 0.209 3934.0 / PLOG / 1.00E+01 3.450E+13 -0.726 6944.0 / PLOG / 1.00E+02 3.310E+14 -0.866 10966.0 / PLOG / 1.00E+03 1.650E+01 3.170 9400.0 / C3H5-A+CH3O2=C3H5O+CH3O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 3.330E+12 -0.158 -1417.0 / PLOG / 1.00E-01 1.660E+14 -0.642 -349.0 / PLOG / 1.00E+00 2.600E+17 -1.520 2379.0 / PLOG / 1.00E+01 9.780E+14 -0.684 3615.0 / PLOG / 1.00E+02 5.470E+03 2.740 1144.0 / C3H5-A+CH3O2=AC4H7OOH 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.910E+31 -7.230 1336.0 / PLOG / 1.00E-01 6.310E+42 -10.300 5569.0 / PLOG / 1.00E+00 1.030E+45 -10.600 7852.0 / PLOG / 1.00E+01 2.790E+37 -7.920 6498.0 / PLOG / 1.00E+02 3.400E+29 -5.280 4540.0 / AC4H7OOH=C3H5O+CH3O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.490E+58 -13.900 54267.0 / PLOG / 1.00E-01 1.800E+54 -12.400 54194.0 / PLOG / 1.00E+00 3.360E+46 -9.810 52468.0 / PLOG / 1.00E+01 2.390E+36 -6.540 49429.0 / PLOG / 1.00E+02 2.560E+27 -3.610 46333.0 / C3H6+OH=C3H5OH+H 2.290E+13 0.070 10580.0 PLOG / 1.30E-03 2.670E+13 0.050 10611.0 / PLOG / 1.00E-02 2.750E+13 0.050 10623.0 / PLOG / 1.30E-02 2.870E+13 0.040 10634.0 / PLOG / 2.50E-02 1.590E+14 -0.160 11125.0 / PLOG / 1.00E-01 3.100E+14 -0.220 11407.0 / PLOG / 1.32E-01 3.780E+14 -0.240 11458.0 / PLOG / 1.00E+00 9.150E+07 1.420 10087.0 / PLOG / 1.00E+01 3.660E+05 2.140 10410.0 / PLOG / 1.00E+02 8.190E+02

2.840 10481.0 / C3H6+OH=C2H3OH+CH3 1.290E+06 1.650 1233.0 PLOG / 1.30E-03 1.290E+06 1.650 1233.0 / PLOG / 1.00E-02 1.820E+04 2.100 1162.0 / PLOG / 1.30E-02 2.040E+03 2.480 1128.0 / PLOG / 2.50E-02 2.880E+02 2.800 1152.0 / PLOG / 1.00E-01 1.400E+01 3.210 1208.0 / PLOG / 1.32E-01 7.710E+00 3.290 1216.0 / PLOG / 1.00E+00 1.130E+04 2.500 3238.0 / PLOG / 1.00E+01 2.410E+19 -1.740 13107.0 / PLOG / 1.00E+02 3.300E-01 3.700 3665.0 / C3H6+OH=IC3H5OH+H 2.870E+00 2.920 625.0 PLOG / 1.30E-03 2.870E+00 2.920 625.0 / PLOG / 1.00E-02 4.840E-01 2.980 704.0 / PLOG / 1.30E-02 3.130E-01 3.040 721.0 / PLOG / 2.50E-02 9.330E-03 3.620 677.0 / PLOG / 1.00E-01 4.640E-05 4.480 687.0 / PLOG / 1.32E-01 2.710E-05 4.560 707.0 / PLOG / 1.00E+00 7.650E-07 5.050 874.0 / PLOG / 1.00E+01 2.640E+15 -0.800 12728.0 / PLOG / 1.00E+02 4.870E-04 4.320 4020.0 / C3H6+OH=SC3H5OH+H 2.870E+00 2.920 625.0 PLOG / 1.30E-03 3.470E+06 1.530 4288.0 / PLOG / 1.00E-02 1.080E+07 1.340 4576.0 / PLOG / 1.30E-02 9.760E+06 1.330 4589.0 / PLOG / 2.50E-02 5.140E+06 1.360 4594.0 / PLOG / 1.00E-01 3.130E+05 1.690 4603.0 / PLOG / 1.32E-01 1.390E+05 1.800 4603.0 / PLOG / 1.00E+00 1.030E+02 2.830 4530.0 / PLOG / 1.00E+01 3.400E-02 3.890 4390.0 / PLOG / 1.00E+02 4.460E-06 5.030 4132.0 / C3H6+OH=CH3CHO+CH3 6.930E+05 1.490 -536.0 PLOG / 1.30E-03 6.930E+05 1.490 -536.0 / PLOG / 1.00E-02 5.940E+03 2.010 -560.0 / PLOG / 1.30E-02 1.100E+03 2.220 -680.0 / PLOG / 2.50E-02 1.070E+02 2.500 -759.0 / PLOG / 1.00E-01 7.830E-01 3.100 -919.0 / PLOG / 1.32E-01 3.070E-01 3.220 -946.0 / PLOG / 1.00E+00 3.160E-04 4.050 -1144.0 / PLOG / 1.00E+01 7.590E-06 4.490 -680.0 / PLOG / 1.00E+02 5.450E-05 4.220 1141.0 / C3H6+OH=C3H6OH1-2 5.100E+54 -20.700 32402.0 PLOG / 1.30E-03 2.300E+78 -20.700 32402.0 / PLOG / 1.00E-02 2.740E+77 -20.000 33874.0 / PLOG / 1.30E-02 1.070E+76 -19.580 32874.0 / PLOG / 2.50E-02 3.680E+73 -18.790 31361.0 / PLOG / 1.00E-01 1.040E+68 -17.010 27909.0 / PLOG / 1.32E-01 7.230E+66 -16.640 27162.0 / PLOG / 1.00E+00 1.950E+59 -14.170 23079.0 / PLOG / 1.00E+01 7.580E+53 -12.230 22976.0 / PLOG / 1.00E+02 1.430E+48 -10.230 23772.0 / DUP C3H6+OH=C3H6OH1-2 1.420E+36 -15.840 11594.0 PLOG / 1.30E-03 6.410E+59 -15.840 11594.0 / PLOG / 1.00E-02 7.280E+59 -15.510 12898.0 / PLOG / 1.30E-02 2.790E+59 -15.340 12913.0 / PLOG / 2.50E-02 2.650E+58 -14.930 12936.0 / PLOG / 1.00E-01 1.350E+56 -14.040 12945.0 / PLOG / 1.32E-01 3.980E+55 -13.850 12887.0 / PLOG / 1.00E+00 1.550E+50 -12.040 11493.0 / PLOG / 1.00E+01 6.410E+41 -9.350 8921.0 / PLOG / 1.00E+02 2.300E+32 -6.310 6088.0 / DUP C3H6+OH=C3H6OH2-1 5.100E+54 -20.700 32402.0 PLOG / 1.30E-03 2.140E+59 -15.840 11594.0 / PLOG / 1.00E-02 2.430E+59 -15.510 12898.0 / PLOG / 1.30E-02 9.300E+58 -15.340 12913.0 / PLOG / 2.50E-02 8.830E+57 -14.930 12936.0 / PLOG / 1.00E-01 4.500E+55 -14.040 12945.0 / PLOG / 1.32E-01 1.330E+55 -13.850 12887.0 / PLOG / 1.00E+00 5.180E+49 -12.040 11493.0 / PLOG / 1.00E+01 2.140E+41 -9.350 8921.0 / PLOG / 1.00E+02 7.650E+31 -6.310 6088.0 / DUP C3H6+OH=C3H6OH2-1 1.420E+36 -15.840 11594.0 PLOG / 1.30E-03 7.680E+77 -20.700 32402.0 / PLOG / 1.00E-02 9.130E+76 -20.000 33874.0 / PLOG /

1.30E-02 3.550E+75 -19.580 32874.0 / PLOG / 2.50E-02 1.230E+73 -18.790 31361.0 / PLOG /
1.00E-01 3.450E+67 -17.010 27909.0 / PLOG / 1.32E-01 2.410E+66 -16.640 27162.0 / PLOG /
1.00E+00 6.500E+58 -14.170 23079.0 / PLOG / 1.00E+01 2.530E+53 -12.230 22976.0 / PLOG
/ 1.00E+02 4.780E+47 -10.230 23772.0 / DUP CH2CCH2OH+H=C3H5OH 1.000E+14 0.000
0.0 C3H5OH+H=CH2CCH2OH+H2 3.900E+05 2.500 5821.0 C3H5OH+O2=CH2CCH2OH+HO2
4.000E+13 0.000 60690.0 C3H5OH+OH=CH2CCH2OH+H2O 5.060E+12 0.000 5960.0 C3H5OH+CH3=CH2CCH2
2.400E+11 0.000 8030.0 CH2CCH2OH+H2O2=C3H5OH+HO2 3.010E+09 0.000 2583.0 CH2CCH2OH=C2H2+CH
2.160E+40 -8.310 45110.0 CH2CCH2OH=CH2O+C2H3 9.240E+10 0.870 30460.0 CH2CCH2OH=C2H3CHO+H
1.110E+11 0.480 36770.0 CH2CCH2OH=HCO+C2H4 9.240E+10 0.870 30460.0 CH2CCH2OH+O2=¿CH2OH+CO
4.340E+12 0.000 0.0 C3H5O+O2=C2H3CHO+HO2 1.000E+12 0.000 6000.0 CH3COCH3+H=C3H6OH2-
1 8.000E+12 0.000 9500.0 IC3H5OH+H=C3H6OH2-1 6.250E+11 0.510 4020.0 C2H5CHO+H=C3H6OH1-
2 8.000E+12 0.000 9500.0 C3H5-T+OH=IC3H5OH 5.000E+13 0.000 0.0 C3H6OH2-1+O2=CH3COCH3+HO2
1.500E+12 0.000 5000.0 C3H6OH1-2+O2=C2H5CHO+HO2 1.500E+12 0.000 5000.0 C3H6OH1-
2+O2=HOC3H6O2 1.200E+11 0.000 -1100.0 C3H6OH2-1+O2=HOC3H6O2 1.200E+11 0.000 -
1100.0 HOC3H6O2=¿CH3CHO+CH2O+OH 1.250E+10 0.000 18900.0 SC3H5OH=C2H5CHO 8.590E+11
0.318 55900.0 SC3H5OH+O2=¿C2H3CHO+H+HO2 3.000E+13 0.000 39100.0 SC3H5OH+OH=¿C2H3CHO+H+H
3.100E+06 2.000 -298.0 SC3H5OH+H=¿C2H3CHO+H+H2 1.730E+05 2.500 2492.0 SC3H5OH+O=¿C2H3CHO+
1.750E+12 0.700 5884.0 SC3H5OH+HO2=¿C2H3CHO+H+H2O2 9.600E+03 2.600 13900.0 SC3H5OH+CH3=¿C2
2.210E+00 3.500 5675.0 SC3H5OH+CH3O2=¿C2H3CHO+H+CH3O2H 9.600E+03 2.600 13900.0
SC3H5OH+CH3O=¿C2H3CHO+H+CH3OH 8.300E+10 0.000 2600.0 SC3H5OH+HO2=C2H5CHO+HO2
1.490E+05 1.670 6810.0 SC3H5OH+HOCHO=C2H5CHO+HOCHO 2.810E-02 3.286 -4509.0 C2H+CH3=C3H4-
P 8.000E+13 0.000 0.0 C3H4-A=C3H4-P 4.790E+48 -10.000 88685.0 PLOG / 1.00E+00 7.760E+39
-7.800 78446.0 / PLOG / 1.00E+01 4.790E+48 -10.000 88685.0 / CC3H4=C3H4-P 1.660E+37 -
7.240 48013.0 PLOG / 3.95E-02 2.510E+50 -11.820 50914.0 / PLOG / 1.00E+00 1.230E+37
-7.510 45551.0 / PLOG / 1.00E+01 1.660E+37 -7.240 48013.0 / CC3H4=C3H4-A 5.010E+35
-6.870 51298.0 PLOG / 3.95E-02 9.770E+43 -9.970 56007.0 / PLOG / 1.00E+00 2.510E+26 -
4.560 43922.0 / PLOG / 1.00E+01 5.010E+35 -6.870 51298.0 / C3H4-P=C3H3+H 6.480E+30
-4.655 93925.0 PLOG / 1.00E+00 6.480E+30 -4.655 93925.0 / PLOG / 1.00E+01 1.210E+25
-2.787 92376.0 / C3H4-A=C3H3+H 1.320E+31 -4.749 92080.0 PLOG / 1.00E+00 1.320E+31 -
4.749 92080.0 / PLOG / 1.00E+01 3.650E+25 -2.950 90625.0 / C3H3+H=CC3H4 3.240E+18
-2.050 2053.0 PLOG / 3.95E-02 8.910E+112 -28.260 83611.0 / PLOG / 1.00E+00 1.070E+21
-2.950 2687.0 / PLOG / 1.00E+01 3.240E+18 -2.050 2053.0 / C3H4-P+C3H3=C3H4-A+C3H3
6.140E+06 1.740 10450.0 C3H4-P+O2=C3H3+HO2 3.000E+13 0.000 42630.0 C3H4-P+O=C3H3+OH
7.650E+08 1.500 8600.0 C3H4-P+H=C3H3+H2 3.570E+04 2.825 4821.0 C3H4-P+OH=C3H3+H2O
4.940E+06 2.027 1060.0 C3H4-P+HO2=C3H3+H2O2 9.550E-02 4.170 9633.0 C3H4-P+CH3=C3H3+CH4
1.800E+12 0.000 7700.0 C3H4-P+CH3O2=C3H3+CH3O2H 9.550E-02 4.170 9633.0 C3H4-P+C2H=C2H2+C3H3

1.000E+13 0.000 0.0 C3H4-P+C2H3=C3H3+C2H4 1.000E+12 0.000 7700.0 C3H4-P+C3H5-A=C3H3+C3H6
3.000E+12 0.000 7700.0 C3H4-A+H=C3H3+H2 6.620E+03 3.095 5522.0 C3H4-A+O2=C3H3+HO2
4.000E+13 0.000 41320.0 C3H4-A+OH=C3H3+H2O 1.480E+05 2.492 1807.0 C3H4-A+CH3=C3H3+CH4
1.300E+12 0.000 7700.0 C3H4-A+HO2=C3H3+H2O2 3.580E-02 4.170 9633.0 C3H4-A+CH3O2=C3H3+CH3O2H
7.160E-02 4.170 9633.0 C3H4-A+C3H5-A=C3H3+C3H6 2.000E+11 0.000 7700.0 C3H4-A+H=C3H4-
P+H 2.440E+10 1.040 2159.0 PLOG / 1.00E-03 8.490E+10 0.890 2503.0 / PLOG / 3.90E-02
1.480E+13 0.260 4103.0 / PLOG / 1.00E+00 2.480E+15 -0.330 6436.0 / PLOG / 1.00E+01
2.350E+25 -3.230 13165.0 / PLOG / 1.00E+02 1.020E+24 -2.670 15552.0 / DUP C3H4-A+H=C3H4-
P+H 2.440E+10 1.040 2159.0 PLOG / 1.00E-03 1.000E-10 0.000 0.0 / PLOG / 3.90E-02 1.000E-10
0.000 0.0 / PLOG / 1.00E+00 1.000E-10 0.000 0.0 / PLOG / 1.00E+01 1.790E+07 1.980 4521.0
/ PLOG / 1.00E+02 4.630E+04 2.620 4466.0 / DUP C3H4-A+H=C3H5-A 2.210E+61 -15.250
20076.0 PLOG / 1.00E-03 2.210E+61 -15.250 20076.0 / PLOG / 3.90E-02 1.240E+52 -12.020
17839.0 / PLOG / 1.00E+00 4.670E+51 -11.450 21340.0 / PLOG / 1.00E+01 3.750E+48 -10.270
22511.0 / PLOG / 1.00E+02 4.230E+43 -8.610 22522.0 / DUP C3H4-A+H=C3H5-A 2.210E+61
-15.250 20076.0 PLOG / 1.00E-03 2.800E+38 -8.670 8035.0 / PLOG / 3.90E-02 9.330E+36 -8.190
7462.0 / PLOG / 1.00E+00 3.320E+30 -5.780 6913.0 / PLOG / 1.00E+01 2.290E+26 -4.320
6163.0 / PLOG / 1.00E+02 4.380E+21 -2.710 5187.0 / DUP C3H4-A+H=C3H5-S 1.100E+30 -
6.520 15200.0 PLOG / 1.00E-01 1.100E+30 -6.520 15200.0 / PLOG / 1.00E+00 5.400E+29 -6.090
16300.0 / PLOG / 1.00E+01 2.600E+31 -6.230 18700.0 / PLOG / 1.00E+02 3.200E+31 -5.880
21500.0 / C3H4-A+H=C3H5-T 6.440E+102 -27.510 51768.0 PLOG / 1.00E-03 6.440E+102 -27.510
51768.0 / PLOG / 3.90E-02 1.550E+53 -13.100 14472.0 / PLOG / 1.00E+00 1.900E+53 -12.590
16726.0 / PLOG / 1.00E+01 7.950E+51 -11.820 18286.0 / PLOG / 1.00E+02 4.210E+52 -11.640
22262.0 / DUP C3H4-A+H=C3H5-T 6.440E+102 -27.510 51768.0 PLOG / 1.00E-03 1.100E+54
-14.290 10809.0 / PLOG / 3.90E-02 9.880E+44 -11.210 8212.0 / PLOG / 1.00E+00 2.810E+40
-9.420 7850.0 / PLOG / 1.00E+01 2.600E+35 -7.570 7147.0 / PLOG / 1.00E+02 9.880E+29 -
5.530 6581.0 / DUP C3H4-A+H=CH3+C2H2 3.740E+01 3.350 58.0 PLOG / 1.00E-03 1.230E+08
1.530 4737.0 / PLOG / 3.90E-02 2.720E+09 1.200 6834.0 / PLOG / 1.00E+00 1.260E+20 -1.830
15003.0 / PLOG / 1.00E+01 1.680E+16 -0.600 14754.0 / PLOG / 1.00E+02 1.370E+17 -0.790
17603.0 / DUP C3H4-A+H=CH3+C2H2 3.740E+01 3.350 58.0 PLOG / 1.00E-03 1.000E-10 0.000
0.0 / PLOG / 3.90E-02 1.000E-10 0.000 0.0 / PLOG / 1.00E+00 1.230E+04 2.680 6335.0 / PLOG
/ 1.00E+01 3.310E+08 1.140 8886.0 / PLOG / 1.00E+02 1.280E+06 1.710 9774.0 / DUP C3H4-
P+H=C3H5-T 8.850E+51 -13.040 12325.0 PLOG / 1.00E-03 8.850E+51 -13.040 12325.0 / PLOG
/ 3.90E-02 3.170E+52 -12.690 14226.0 / PLOG / 1.00E+00 2.870E+53 -12.510 16853.0 / PLOG
/ 1.00E+01 9.510E+51 -11.740 18331.0 / PLOG / 1.00E+02 4.510E+52 -11.580 22207.0 / DUP
C3H4-P+H=C3H5-T 8.850E+51 -13.040 12325.0 PLOG / 1.00E-03 1.970E+46 -11.910 7456.0 /
PLOG / 3.90E-02 2.590E+45 -11.230 8046.0 / PLOG / 1.00E+00 6.930E+39 -9.110 7458.0 /

PLOG / 1.00E+01 6.800E+34 -7.290 6722.0 / PLOG / 1.00E+02 5.650E+29 -5.390 6150.0 / DUP C3H4-P+H=C3H5-S 3.380E+49 -12.750 14072.0 PLOG / 1.00E-03 1.000E-10 0.000 0.0 / PLOG / 3.90E-02 3.380E+49 -12.750 14072.0 / PLOG / 1.00E+00 1.370E+51 -12.550 15428.0 / PLOG / 1.00E+01 3.880E+50 -11.900 16915.0 / PLOG / 1.00E+02 2.170E+49 -11.100 18746.0 / DUP C3H4-P+H=C3H5-S 3.380E+49 -12.750 14072.0 PLOG / 1.00E-03 1.490E+38 -10.110 7458.0 / PLOG / 3.90E-02 2.980E+43 -11.430 8736.0 / PLOG / 1.00E+00 5.750E+39 -9.510 8772.0 / PLOG / 1.00E+01 4.330E+40 -9.600 9401.0 / PLOG / 1.00E+02 3.440E+34 -7.360 8558.0 / DUP C3H4-P+H=CH3+C2H2 2.120E+10 1.060 3945.0 PLOG / 1.00E-03 2.440E+10 1.040 3980.0 / PLOG / 3.90E-02 3.890E+10 0.989 4114.0 / PLOG / 1.00E+00 3.460E+12 0.442 5463.0 / PLOG / 1.00E+01 1.720E+14 -0.010 7134.0 / PLOG / 1.00E+02 1.900E+15 -0.290 8306.0 / C3H4-P+H=C3H5-A 1.100E+60 -14.560 28100.0 PLOG / 1.00E-01 1.100E+60 -14.560 28100.0 / PLOG / 1.00E+00 4.910E+60 -14.370 31644.0 / PLOG / 2.00E+00 3.040E+60 -14.190 32642.0 / PLOG / 5.00E+00 9.020E+59 -13.890 33953.0 / PLOG / 1.00E+01 2.200E+59 -13.610 34900.0 / PLOG / 1.00E+02 1.600E+55 -12.070 37500.0 / C3H5-A=C3H5-T 3.900E+59 -15.420 75400.0 PLOG / 1.00E-01 3.900E+59 -15.420 75400.0 / PLOG / 1.00E+00 7.060E+56 -14.080 75868.0 / PLOG / 2.00E+00 4.800E+55 -13.590 75949.0 / PLOG / 5.00E+00 4.860E+53 -12.810 75883.0 / PLOG / 1.00E+01 6.400E+51 -12.120 75700.0 / PLOG / 1.00E+02 2.800E+43 -9.270 74000.0 / C3H5-A=C3H5-S 1.300E+55 -14.530 73800.0 PLOG / 1.00E-01 1.300E+55 -14.530 73800.0 / PLOG / 1.00E+00 5.000E+51 -13.020 73300.0 / PLOG / 1.00E+01 9.700E+48 -11.730 73700.0 / PLOG / 1.00E+02 4.860E+44 -9.840 73400.0 / C2H2+CH3=C3H5-T 6.800E+20 -4.160 18000.0 PLOG / 1.00E-01 6.800E+20 -4.160 18000.0 / PLOG / 1.00E+00 4.990E+22 -4.390 18850.0 / PLOG / 2.00E+00 6.000E+23 -4.600 19571.0 / PLOG / 5.00E+00 7.310E+25 -5.060 21150.0 / PLOG / 1.00E+01 9.300E+27 -5.550 22900.0 / PLOG / 1.00E+02 3.800E+36 -7.580 31300.0 / C3H5-T=C3H5-S 1.600E+44 -12.160 52200.0 PLOG / 1.00E-01 1.600E+44 -12.160 52200.0 / PLOG / 1.00E+00 1.500E+48 -12.710 53900.0 / PLOG / 1.00E+01 5.100E+52 -13.370 57200.0 / PLOG / 1.00E+02 5.800E+51 -12.430 59200.0 / C2H2+CH3=C3H5-A 8.200E+53 -13.320 33200.0 PLOG / 1.00E-01 8.200E+53 -13.320 33200.0 / PLOG / 1.00E+00 2.680E+53 -12.820 35730.0 / PLOG / 2.00E+00 3.640E+52 -12.460 36127.0 / PLOG / 5.00E+00 1.040E+51 -11.890 36476.0 / PLOG / 1.00E+01 4.400E+49 -11.400 36700.0 / PLOG / 1.00E+02 3.800E+44 -9.630 37600.0 / CH3+C2H2=C3H5-S 1.780E+42 -10.400 13647.0 PLOG / 1.00E-03 1.780E+42 -10.400 13647.0 / PLOG / 3.90E-02 1.520E+44 -10.730 15256.0 / PLOG / 1.00E+00 1.190E+44 -10.190 18728.0 / PLOG / 1.00E+01 6.020E+43 -9.740 20561.0 / PLOG / 1.00E+02 1.420E+42 -8.910 22235.0 / DUP CH3+C2H2=C3H5-S 1.780E+42 -10.400 13647.0 PLOG / 1.00E-03 1.000E-10 0.000 0.0 / PLOG / 3.90E-02 1.000E-10 0.000 0.0 / PLOG / 1.00E+00 8.490E+35 -8.430 12356.0 / PLOG / 1.00E+01 3.040E+32 -7.010 12357.0 / PLOG / 1.00E+02 1.690E+27 -5.070 11690.0 / DUP C3H4-P+O=HCCO+CH3 7.300E+12 0.000 2250.0 C3H4-P+O=C2H4+CO 1.000E+13 0.000 2250.0

C3H4-P+O=C2H3+HCO 3.200E+12 0.000 2010.0 C3H4-A+O=C2H4+CO 2.000E+07 1.800 1000.0
C3H4-A+O=C2H2+CH2O 3.000E-03 4.610 -4243.0

C3H4-A+OH=CH2CCH2OH 1.110E+12 0.000 -304.0 C3H4-A+OH=SC3H4OH 2.220E+12 0.000
-304.0 SC3H4OH=CH2CO+CH3 9.240E+10 0.870 30460.0

C3H4-P+OH=PC3H4OH-2 3.930E+11 0.000 0.0 C3H4-P+OH=SC3H4OH 2.360E+12 0.000
0.0 PC3H4OH-2=CH3CHCHO 3.560E+10 0.880 23238.0 CH3CHCHO=C2H3CHO+H 1.000E+00
1.000 1.0 PLOG / 1.00E-02 1.740E+50 -11.730 52870.0 / PLOG / 1.00E-01 1.130E+47 -10.570
50479.0 / PLOG / 1.00E+00 2.940E+43 -9.290 48810.0 / PLOG / 2.50E+00 1.160E+42 -8.780
48382.0 / PLOG / 5.00E+00 9.480E+40 -8.400 48095.0 / PLOG / 1.00E+01 7.190E+39 -8.010
47818.0 / PLOG / 2.50E+01 2.130E+38 -7.490 47438.0 / PLOG / 5.00E+01 1.420E+37 -7.090
47128.0 / CH3CHCHO=CH3CHCO+H 8.330E+12 -0.020 32410.0 CH3CHCHO+H2=C2H5CHO+H
2.160E+05 2.380 18990.0 C3H4-P+HO2=¿C2H4+CO+OH 3.000E+12 0.000 19000.0 C3H4-A+HO2=¿C2H4+CO-
1.000E+11 0.000 14000.0 C3H4-A+HO2=¿CH2CO+CH2+OH 4.000E+12 0.000 19000.0 C3H4-
A+C2H=C2H2+C3H3 1.000E+13 0.000 0.0 C3H3+O=CH2O+C2H 2.000E+13 0.000 0.0 C3H3+HO2=¿OH+CO+
8.000E+11 0.000 0.0 C3H3+HCO=C3H4-A+CO 2.500E+13 0.000 0.0 C3H3+HCO=C3H4-P+CO
2.500E+13 0.000 0.0 C2H5+C2H=C3H3+CH3 1.810E+13 0.000 0.0 C3H3+O2=CH2CO+HCO
1.700E+05 1.700 1500.0 C3H3+CH=C4H3-N+H 7.000E+13 0.000 0.0 C3H3+HO2=C3H3O+OH
1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.020E+13 -0.158 -1417.0 / PLOG / 1.00E-01 4.980E+14
-0.642 -349.0 / PLOG / 1.00E+00 7.770E+17 -1.520 2379.0 / PLOG / 1.00E+01 2.930E+15 -
0.684 3615.0 / PLOG / 1.00E+02 1.640E+04 2.740 1144.0 / C3H3+HO2=C3H3O2H 1.000E+11
0.000 0.0 PLOG / 1.00E-02 1.910E+31 -7.230 1336.0 / PLOG / 1.00E-01 6.310E+42 -10.300
5569.0 / PLOG / 1.00E+00 1.030E+45 -10.600 7852.0 / PLOG / 1.00E+01 2.790E+37 -7.920
6498.0 / PLOG / 1.00E+02 4.730E+25 -4.130 2924.0 / C3H3+HO2=C2HCHO+H2O 1.000E+11
0.000 0.0 PLOG / 1.00E-02 1.090E+00 3.010 -3421.0 / PLOG / 1.00E-01 6.350E+01 2.500 -
2341.0 / PLOG / 1.00E+00 6.050E+05 1.390 595.0 / PLOG / 1.00E+01 3.100E+05 1.590 2678.0
/ PLOG / 1.00E+02 5.070E-05 4.590 928.0 / C3H3O2H=C2HCHO+H2O 1.000E+11 0.000 0.0
PLOG / 1.00E-02 1.990E+50 -12.700 53532.0 / PLOG / 1.00E-01 4.720E+47 -11.500 54361.0 /
PLOG / 1.00E+00 1.500E+40 -8.840 53179.0 / PLOG / 1.00E+01 2.540E+28 -5.000 49919.0
/ PLOG / 1.00E+02 1.480E+16 -1.120 45949.0 / C2H+CH2O=C3H3O 1.000E+11 0.000 0.0
PLOG / 1.00E-03 5.930E-04 2.609 -4297.0 / PLOG / 1.00E-02 5.690E+06 -0.073 -1234.0 /
PLOG / 1.00E-01 5.390E+13 -1.803 1452.0 / PLOG / 1.00E+00 8.730E+15 -2.074 2510.0 /
PLOG / 1.00E+01 5.300E+19 -2.943 4532.0 / PLOG / 1.00E+02 3.780E+21 -3.163 6802.0
/ C2HCHO=C2H2+CO 2.510E+14 0.000 68000.0 C2H+HCO=C2HCHO 1.000E+13 0.000 0.0
C3H3+H=C3H2+H2 2.140E+05 2.520 7453.0 C3H3+H=C3H2(S)+H2 3.310E+13 0.195 17579.0
PLOG / 3.95E-02 2.950E+09 1.280 13474.0 / PLOG / 1.00E+00 1.100E+10 1.130 13929.0 / PLOG

/ 1.00E+01 3.310E+13 0.195 17579.0 / C3H3+H=H2CCC(S)+H2 1.000E+18 -1.230 15111.0
PLOG / 3.95E-02 2.690E+09 1.050 5371.0 / PLOG / 1.00E+00 2.880E+13 -0.030 9448.0 /
PLOG / 1.00E+01 1.000E+18 -1.230 15111.0 / C3H3+H=C3H2C+H2 7.240E+09 0.606 18356.0
PLOG / 3.95E-02 1.070E+07 1.370 15557.0 / PLOG / 1.00E+00 1.350E+07 1.340 15560.0 /
PLOG / 1.00E+01 7.240E+09 0.606 18356.0 / C3H2C+O2=C2H2+CO2 1.000E+13 0.000 0.0
C3H3+OH=C3H2+H2O 2.000E+13 0.000 8000.0 C3H3+OH=CH2O+C2H2 2.000E+12 0.000 0.0
C3H3+OH=C2H3+HCO 1.000E+13 0.000 0.0 C3H3+OH=C2H4+CO 1.000E+13 0.000 0.0 C3H3+OH=C3H2(S)+
1.000E+12 0.000 0.0 C3H3+OH=H2CCC(S)+H2O 1.000E+12 0.000 0.0 C3H2(S)+M=C3H2+M
1.000E+13 0.000 0.0 C3H2(S)+H=H2CCC(S)+H 1.000E+13 0.000 0.0 H2CCC(S)+O2=CO2+C2H2
1.000E+13 0.000 0.0 C3H3+C3H3=C6H5+H 1.050E+54 -11.880 28757.0 PLOG / 3.95E-02 1.050E+54
-11.880 28757.0 / PLOG / 1.00E+00 1.700E+48 -9.977 36755.0 / PLOG / 1.00E+01 3.670E+26
-3.879 28963.0 / C3H3+C3H3=C6H6 1.820E+74 -18.140 31896.0 PLOG / 3.95E-02 1.640E+66
-15.902 27529.0 / PLOG / 1.00E+00 3.160E+55 -12.550 22264.0 / PLOG / 1.00E+01 3.890E+50 -
11.010 20320.0 / C3H3+C3H3=FULVENE 6.310E+76 -19.070 31542.0 PLOG / 3.95E-02 7.250E+65
-16.015 25035.0 / PLOG / 1.00E+00 1.380E+66 -15.660 28260.0 / PLOG / 1.00E+01 1.260E+56 -
12.610 23515.0 / C3H3+C3H5-A=¿FULVENE+H+H 3.260E+29 -5.397 3390.0 C3H3+C3H4-A=C6H6+H
1.400E+12 0.000 9990.0 CH3CHCO+OH=C2H5+CO2 1.730E+12 0.000 -1010.0 CH3CHCO+OH=SC2H4OH+CO
2.000E+12 0.000 -1010.0 CH3CHCO+H=C2H5+CO 4.400E+12 0.000 1459.0 CH3CHCO+O=CH3CHO+CO
3.200E+12 0.000 -437.0

CH3COCH3=CH3CO+CH3 2.050E+58 -12.796 100030.0 PLOG / 1.00E-02 2.050E+58 -12.796
100030.0 / PLOG / 1.00E-01 3.300E+51 -10.574 98221.0 / PLOG / 1.00E+00 1.310E+42 -7.657
94661.0 / PLOG / 1.00E+01 2.160E+33 -4.989 90916.0 / PLOG / 1.00E+02 9.400E+28 -3.669
89023.0 / CH3COCH2+H=CH3COCH3 1.000E+13 0.000 0.0 CH3COCH3+OH=CH3COCH2+H2O
1.250E+05 2.483 445.0 CH3COCH3+H=CH3COCH2+H2 9.800E+05 2.430 5160.0 CH3COCH3+O=CH3COCH2+
5.130E+11 0.211 4890.0 CH3COCH3+CH3=CH3COCH2+CH4 3.960E+11 0.000 9784.0 CH3COCH3+CH3O=CH3
4.340E+11 0.000 6460.0 CH3COCH3+O2=CH3COCH2+HO2 6.030E+13 0.000 48500.0 CH3COCH3+HO2=CH3C
1.700E+13 0.000 20460.0 CH3COCH3+CH3O2=CH3COCH2+CH3O2H 1.700E+13 0.000 20460.0
CH3COCH3+CH3COCH2O2=CH3COCH2+C3KET21 1.000E+11 0.000 5000.0 CH3COCH2+HO2=CH3COCH2O-
2.410E+13 0.000 0.0 CH3COCH2+CH3O2=CH3COCH2O+CH3O 1.200E+13 0.000 0.0 CH3COCH2O=CH3CO+C
5.870E+20 -2.422 10536.0 CH3COCH2+O2=CH3COCH2O2 1.200E+11 0.000 -1100.0 CH2CO+CH3=CH3COCH2
1.760E+04 2.480 6130.0 CH2O+CH3COCH2O2=HCO+C3KET21 1.290E+11 0.000 9000.0 HO2+CH3COCH2O2=
1.000E+12 0.000 0.0 C2H3+HCO=C2H3CHO 1.810E+13 0.000 0.0 C2H3CHO+H=C2H3CO+H2
1.340E+13 0.000 3300.0 C2H3CHO+O=C2H3CO+OH 5.940E+12 0.000 1868.0 C2H3CHO+OH=C2H3CO+H2O
9.240E+06 1.500 -962.0 C2H3CHO+O2=C2H3CO+HO2 1.000E+13 0.000 40700.0 C2H3CHO+HO2=C2H3CO+H
3.010E+12 0.000 11920.0 C2H3CHO+CH3=C2H3CO+CH4 2.610E+06 1.780 5911.0 C2H3CHO+C2H3=C2H3CO+

1.740E+12 0.000 8440.0 C2H3CHO+CH3O=C2H3CO+CH3OH 1.000E+12 0.000 3300.0 C2H3CHO+CH3O2=C2H

3.010E+12 0.000 11920.0 C2H3+CO=C2H3CO 1.510E+11 0.000 4810.0 C2H5+HCO=C2H5CHO

1.810E+13 0.000 0.0 C2H5CHO+H=C2H5CO+H2 4.000E+13 0.000 4200.0 C2H5CHO+O=C2H5CO+OH

5.000E+12 0.000 1790.0 C2H5CHO+OH=C2H5CO+H2O 2.690E+10 0.760 -340.0 C2H5CHO+CH3=C2H5CO+CH

2.610E+06 1.780 5911.0 C2H5CHO+HO2=C2H5CO+H2O2 2.800E+12 0.000 13600.0 C2H5CHO+CH3O=C2H5C

1.000E+12 0.000 3300.0 C2H5CHO+CH3O2=C2H5CO+CH3O2H 3.010E+12 0.000 11920.0 C2H5CHO+C2H5=C2

1.000E+12 0.000 8000.0 C2H5CHO+C2H5O=C2H5CO+C2H5OH 6.030E+11 0.000 3300.0 C2H5CHO+C2H5O2=

3.010E+12 0.000 11920.0 C2H5CHO+O2=C2H5CO+HO2 1.000E+13 0.000 40700.0 C2H5CHO+CH3CO3=C2H5C

3.010E+12 0.000 11920.0 C2H5CHO+C2H3=C2H5CO+C2H4 1.700E+12 0.000 8440.0 C2H5CHO+NC3H7=C2H5

1.700E+12 0.000 8440.0 C2H5CHO+IC3H7=C2H5CO+C3H8 1.700E+12 0.000 8440.0 C2H5CHO+C3H5-

A=C2H5CO+C3H6 1.700E+12 0.000 8440.0 C2H5+CO=C2H5CO 1.510E+11 0.000 4810.0 C4H10(+M)=C2H5+C

1.360E+37 -6.036 92929.0 LOW / 4.720E+18 0.000 49578.0 / TROE / 7.998E-02 1.000E-20

3.243E+04 4.858E+03 / C4H10(+M)=NC3H7+CH3(+M) 6.600E+52 -10.626 100330.0 LOW /

5.340E+17 0.000 42959.0 / TROE / 9.502E-02 1.000E-20 5.348E+03 4.326E+03 / C4H10=PC4H9+H

4.800E+40 -7.060 115302.0 PLOG / 1.00E-02 4.450E+90 -21.910 140564.0 / PLOG / 1.00E-01

4.630E+76 -17.640 134669.0 / PLOG / 1.00E+00 4.940E+58 -12.320 125435.0 / PLOG / 1.00E+01

4.800E+40 -7.060 115302.0 / PLOG / 1.00E+02 1.490E+27 -3.150 107323.0 / C4H10=SC4H9+H

8.520E+38 -6.580 110556.0 PLOG / 1.00E-02 3.100E+88 -21.240 136355.0 / PLOG / 1.00E-01

4.340E+73 -16.760 129590.0 / PLOG / 1.00E+00 7.390E+55 -11.520 120199.0 / PLOG / 1.00E+01

8.520E+38 -6.580 110556.0 / PLOG / 1.00E+02 5.400E+26 -3.050 103313.0 / C4H10+H=PC4H9+H2

3.490E+05 2.690 6450.0 C4H10+O2=PC4H9+HO2 6.000E+13 0.000 52340.0 C4H10+O=PC4H9+OH

1.130E+14 0.000 7850.0 C4H10+OH=PC4H9+H2O 1.050E+10 0.970 1586.0 C4H10+HO2=PC4H9+H2O2

4.080E+01 3.590 17160.0 C4H10+CH3=PC4H9+CH4 9.040E-01 3.650 7154.0 C4H10+CH3O=PC4H9+CH3OH

3.000E+11 0.000 7000.0 C4H10+CH3O2=PC4H9+CH3O2H 1.390E+00 3.970 18280.0 C4H10+O2CHO=PC4H9+

1.680E+13 0.000 20440.0 C4H10+C2H5=PC4H9+C2H6 1.580E+11 0.000 12300.0 C4H10+C2H3=PC4H9+C2H4

1.000E+12 0.000 18000.0 C4H10+C2H5O=PC4H9+C2H5OH 3.000E+11 0.000 7000.0 C4H10+C2H5O2=PC4H9+

4.080E+01 3.590 17160.0 C4H10+CH3CO3=PC4H9+CH3CO3H 1.700E+13 0.000 20460.0 C4H10+C3H5-

A=PC4H9+C3H6 7.940E+11 0.000 20500.0 C4H10+NC3H7O2=PC4H9+NC3H7O2H 1.700E+13

0.000 20460.0 C4H10+IC3H7O2=PC4H9+IC3H7O2H 1.700E+13 0.000 20460.0 C4H10+PC4H9=SC4H9+C4H10

1.000E+11 0.000 10400.0 C4H10+PC4H9O2=PC4H9+PC4H9O2H 1.700E+13 0.000 20460.0 C4H10+SC4H9O2=P

1.700E+13 0.000 20460.0 C4H10+IC4H9O2=PC4H9+IC4H9O2H 1.700E+13 0.000 20460.0 C4H10+TC4H9O2=PC

1.700E+13 0.000 20460.0 C4H10+H=SC4H9+H2 2.600E+06 2.400 4471.0 C4H10+O2=SC4H9+HO2

4.000E+13 0.000 49800.0 C4H10+O=SC4H9+OH 5.620E+13 0.000 5200.0 C4H10+OH=SC4H9+H2O

9.340E+07 1.610 -35.0 C4H10+HO2=SC4H9+H2O2 1.260E+02 3.370 13720.0 C4H10+CH3=SC4H9+CH4

3.020E+00 3.460 5481.0 C4H10+CH3O=SC4H9+CH3OH 6.000E+11 0.000 7000.0 C4H10+CH3O2=SC4H9+CH3

2.040E+01 3.580 14810.0 C4H10+O2CHO=SC4H9+HO2CHO 1.120E+13 0.000 17690.0 C4H10+C2H5=SC4H9+

1.000E+11 0.000 10400.0 C4H10+C2H3=SC4H9+C2H4 8.000E+11 0.000 16800.0 C4H10+C2H5O=SC4H9+C2H5
6.000E+11 0.000 7000.0 C4H10+C2H5O2=SC4H9+C2H5O2H 1.260E+02 3.370 13720.0 C4H10+CH3CO3=SC4H9
1.120E+13 0.000 17700.0 C4H10+C3H5-A=SC4H9+C3H6 3.160E+11 0.000 16400.0 C4H10+NC3H7O2=SC4H9+
1.120E+13 0.000 17700.0 C4H10+IC3H7O2=SC4H9+IC3H7O2H 1.120E+13 0.000 17700.0 C4H10+PC4H9O2=SC
1.120E+13 0.000 17700.0 C4H10+SC4H9O2=SC4H9+SC4H9O2H 1.120E+13 0.000 17700.0 C4H10+IC4H9O2=SC
1.120E+13 0.000 17700.0 C4H10+TC4H9O2=SC4H9+TC4H9O2H 1.120E+13 0.000 17700.0 PC4H9+HO2=PC4H
7.000E+12 0.000 -1000.0 CH3O2+PC4H9=CH3O+PC4H9O 7.000E+12 0.000 -1000.0 SC4H9+HO2=SC4H9O+OH
7.000E+12 0.000 -1000.0 SC4H9+CH3O2=CH3O+SC4H9O 7.000E+12 0.000 -1000.0 C2H5+CH3CHO=SC4H9O
3.330E+10 0.000 6397.0 PC4H9+O2=C4H8-1+HO2 8.370E-01 3.590 11960.0 PC4H9+O2=PC4H9O2
6.860E+16 -1.627 199.0 SC4H9+O2=C4H8-1+HO2 5.350E-01 3.710 9322.0 SC4H9+O2=C4H8-
2+HO2 1.070E+00 3.710 9322.0 SC4H9+O2=SC4H9O2 3.490E+14 -0.816 -536.0 PC4H9O2+H2=PC4H9O2H+H
3.010E+13 0.000 26030.0 PC4H9O2+HO2=PC4H9O2H+O2 1.750E+10 0.000 -3275.0 PC4H9O2+H2O2=PC4H9O
2.400E+12 0.000 10000.0 PC4H9O2+CH4=PC4H9O2H+CH3 1.120E+13 0.000 24640.0 PC4H9O2+CH3OH=PC4H
6.300E+12 0.000 19360.0 PC4H9O2+CH2O=PC4H9O2H+HCO 5.600E+12 0.000 13600.0 PC4H9O2+C2H6=PC4
1.700E+13 0.000 20460.0 PC4H9O2+CH3CHO=PC4H9O2H+CH3CO 2.800E+12 0.000 13600.0
PC4H9O2+C2H4=PC4H9O2H+C2H3 1.130E+13 0.000 30430.0 PC4H9O2+C3H6=PC4H9O2H+C3H5-
A 5.350E-02 4.207 13288.0 PC4H9O2+C2H5CHO=PC4H9O2H+C2H5CO 2.000E+11 0.000 9500.0
PC4H9O2+C2H3CHO=PC4H9O2H+C2H3CO 2.800E+12 0.000 13600.0 PC4H9O2+C3H8=PC4H9O2H+NC3H7
1.700E+13 0.000 20460.0 PC4H9O2+C3H8=PC4H9O2H+IC3H7 2.000E+12 0.000 17000.0 PC4H9O2+CH3=PC4H
7.000E+12 0.000 -1000.0 PC4H9O2+C2H5=PC4H9O+C2H5O 7.000E+12 0.000 -1000.0 PC4H9O2+IC3H7=PC4H
7.000E+12 0.000 -1000.0 PC4H9O2+NC3H7=PC4H9O+NC3H7O 7.000E+12 0.000 -1000.0 PC4H9O2+C3H5-
A=PC4H9O+C3H5O 7.000E+12 0.000 -1000.0 PC4H9O2+PC4H9=PC4H9O+PC4H9O 7.000E+12
0.000 -1000.0 PC4H9O2+SC4H9=PC4H9O+SC4H9O 7.000E+12 0.000 -1000.0 PC4H9O2+C4H71-
3=PC4H9O+C4H71-O 7.000E+12 0.000 -1000.0 PC4H9O2H=PC4H9O+OH 1.500E+16 0.000
42500.0 PC4H9O2+CH3O2=¿PC4H9O+CH3O+O2 1.400E+16 -1.610 1860.0 PC4H9O2+CH3CO3=¿PC4H9O+C
1.400E+16 -1.610 1860.0 PC4H9O2+C2H5O2=¿PC4H9O+C2H5O+O2 1.400E+16 -1.610 1860.0
PC4H9O2+NC3H7O2=¿PC4H9O+NC3H7O+O2 1.400E+16 -1.610 1860.0 PC4H9O2+IC3H7O2=¿PC4H9O+IC3H
1.400E+16 -1.610 1860.0 PC4H9O2+PC4H9O2=¿PC4H9O+PC4H9O+O2 1.400E+16 -1.610 1860.0
PC4H9O2+SC4H9O2=¿PC4H9O+SC4H9O+O2 1.400E+16 -1.610 1860.0 PC4H9O2=C4H8OOH1-
2 4.010E+08 1.100 30100.0 PC4H9O2=C4H8OOH1-3 1.360E+07 1.300 18200.0 PC4H9O2=C4H8OOH1-
4 1.230E+06 1.500 20000.0 PC4H9O2=C4H8-1+HO2 1.260E+08 1.380 28900.0 IC3H7O2+PC4H9=IC3H7O+PC4H
7.000E+12 0.000 -1000.0 NC3H7O2+PC4H9=NC3H7O+PC4H9O 7.000E+12 0.000 -1000.0 SC4H9O2+PC4H9=SC
7.000E+12 0.000 -1000.0 IC3H7O2+SC4H9=IC3H7O+SC4H9O 7.000E+12 0.000 -1000.0 NC3H7O2+SC4H9=NC3
7.000E+12 0.000 -1000.0 SC4H9O2+H2=SC4H9O2H+H 3.010E+13 0.000 26030.0 SC4H9O2+HO2=SC4H9O2H+
1.750E+10 0.000 -3275.0 SC4H9O2+CH2O=SC4H9O2H+HCO 5.600E+12 0.000 13600.0 SC4H9O2+CH3CHO=SC
2.800E+12 0.000 13600.0 SC4H9O2+C2H6=SC4H9O2H+C2H5 1.700E+13 0.000 20460.0 SC4H9O2+C2H5CHO=

2.000E+11 0.000 9500.0 SC4H9O2+C3H6=SC4H9O2H+C3H5-A 5.350E-02 4.207 13288.0 SC4H9O2+C2H4=SC4H
1.130E+13 0.000 30430.0 SC4H9O2+CH3OH=SC4H9O2H+CH2OH 6.300E+12 0.000 19360.0
SC4H9O2+C2H3CHO=SC4H9O2H+C2H3CO 2.800E+12 0.000 13600.0 SC4H9O2+CH4=SC4H9O2H+CH3
1.120E+13 0.000 24640.0 SC4H9O2+H2O2=SC4H9O2H+HO2 2.400E+12 0.000 10000.0 SC4H9O2+C3H8=SC4H
1.700E+13 0.000 20460.0 SC4H9O2+C3H8=SC4H9O2H+IC3H7 2.000E+12 0.000 17000.0 SC4H9O2+CH3O2=¿S
1.400E+16 -1.610 1860.0 SC4H9O2+CH3CO3=¿SC4H9O+CH3CO2+O2 1.400E+16 -1.610 1860.0
SC4H9O2+NC3H7O2=¿SC4H9O+NC3H7O+O2 1.400E+16 -1.610 1860.0 SC4H9O2+IC3H7O2=¿SC4H9O+IC3H
1.400E+16 -1.610 1860.0 SC4H9O2+SC4H9O2=¿SC4H9O+SC4H9O+O2 1.400E+16 -1.610 1860.0
SC4H9O2+C2H5O2=¿SC4H9O+C2H5O+O2 1.400E+16 -1.610 1860.0 SC4H9O2+CH3=SC4H9O+CH3O
7.000E+12 0.000 -1000.0 SC4H9O2+C2H5=SC4H9O+C2H5O 7.000E+12 0.000 -1000.0 SC4H9O2+IC3H7=SC4H9
7.000E+12 0.000 -1000.0 SC4H9O2+NC3H7=SC4H9O+NC3H7O 7.000E+12 0.000 -1000.0 SC4H9O2+SC4H9=SC
7.000E+12 0.000 -1000.0 SC4H9O2+C3H5-A=SC4H9O+C3H5O 7.000E+12 0.000 -1000.0 SC4H9O2+C4H71-
3=SC4H9O+C4H71-O 7.000E+12 0.000 -1000.0 SC4H9O+OH=SC4H9O2H 1.000E+15 -0.800 0.0
SC4H9O2=C4H8OOH2-1 1.460E+09 1.100 33500.0 SC4H9O2=C4H8OOH2-3 1.720E+09 0.900
29500.0 SC4H9O2=C4H8OOH2-4 1.440E+07 1.400 20800.0 SC4H9O2=C4H8-1+HO2 5.130E+09
1.000 30400.0 C4H8OOH1-2=C4H8O1-2+OH 1.710E+09 1.060 10900.0 C4H8OOH1-3=C4H8O1-
3+OH 2.590E+09 0.690 16000.0 C4H8OOH1-4=C4H8O1-4+OH 1.720E+08 0.760 11100.0 C4H8OOH2-
4=C4H8O1-3+OH 2.440E+09 0.780 18000.0 C4H8O1-2+H=¿CH2O+C3H5-A+H2 5.000E+12 0.000
0.0 C4H8O1-2+O=¿CH2O+C3H5-A+OH 5.000E+12 0.000 0.0 C4H8O1-2+OH=¿CH2O+C3H5-
A+H2O 5.000E+12 0.000 0.0 C4H8O1-2+HO2=¿CH2O+C3H5-A+H2O2 1.000E+13 0.000 15000.0
C4H8O1-2+CH3=¿CH2O+C3H5-A+CH4 2.000E+11 0.000 10000.0 C4H8O1-2+CH3O2=¿CH2O+C3H5-
A+CH3O2H 1.000E+13 0.000 19000.0 C4H8O1-3+H=¿CH2O+C3H5-A+H2 5.000E+12 0.000 0.0
C4H8O1-3+O=¿CH2O+C3H5-A+OH 5.000E+12 0.000 0.0 C4H8O1-3+OH=¿CH2O+C3H5-A+H2O
5.000E+12 0.000 0.0 C4H8O1-3+HO2=¿CH2O+C3H5-A+H2O2 1.000E+13 0.000 15000.0 C4H8O1-
3+CH3=¿CH2O+C3H5-A+CH4 2.000E+11 0.000 10000.0 C4H8O1-3+CH3O2=¿CH2O+C3H5-
A+CH3O2H 1.000E+13 0.000 19000.0 C4H8O1-4+H=¿CH2O+C3H5-A+H2 5.000E+12 0.000 0.0
C4H8O1-4+O=¿CH2O+C3H5-A+OH 5.000E+12 0.000 0.0 C4H8O1-4+OH=¿CH2O+C3H5-A+H2O
5.000E+12 0.000 0.0 C4H8O1-4+HO2=¿CH2O+C3H5-A+H2O2 1.000E+13 0.000 15000.0 C4H8O1-
4+CH3=¿CH2O+C3H5-A+CH4 2.000E+11 0.000 10000.0 C4H8O1-4+CH3O2=¿CH2O+C3H5-
A+CH3O2H 1.000E+13 0.000 19000.0 C4H8O2-3+H=¿CH2O+C3H5-A+H2 5.000E+12 0.000 0.0
C4H8O2-3+OH=¿CH2O+C3H5-A+H2O 5.000E+12 0.000 0.0 C4H8O2-3+O=¿CH2O+C3H5-A+OH
5.000E+12 0.000 0.0 C4H8O2-3+HO2=¿CH2O+C3H5-A+H2O2 1.000E+13 0.000 15000.0 C4H8O2-
3+CH3O2=¿CH2O+C3H5-A+CH3O2H 1.000E+13 0.000 19000.0 C4H8O2-3+CH3=¿CH2O+C3H5-
A+CH4 2.000E+11 0.000 10000.0 CH2CHO+C2H4=C4H7O12-4 1.000E+11 0.000 7800.0 C2H4+CH2CHO=C4H7O
4 1.000E+11 0.000 7800.0 CH3+C2H3CHO=C4H7O23-1 1.000E+11 0.000 7800.0 C4H8OOH1-
3=¿OH+CH2O+C3H6 1.230E+09 1.300 24900.0 C4H8OOH2-4=¿OH+CH3CHO+C2H4 3.080E+08

1.500 23500.0 C4H8OOH1-2+O2=C4H8OOH1-2O2 1.740E+14 -0.816 -536.0 C4H8OOH1-3+O2=C4H8OOH1-3O2 1.740E+14 -0.816 -536.0 C4H8OOH1-4+O2=C4H8OOH1-4O2 3.430E+16 -1.627 199.0 C4H8OOH2-1+O2=C4H8OOH2-1O2 3.430E+16 -1.627 199.0 C4H8OOH2-3+O2=C4H8OOH2-3O2 1.740E+14 -0.816 -536.0 C4H8OOH2-4+O2=C4H8OOH2-4O2 3.430E+16 -1.627 199.0 C4H8OOH1-2O2=C4H72-1OOH+HO2 2.540E+10 0.804 30098.0 C4H8OOH1-3O2=C4H71-4OOH+HO2 5.130E+09 1.000 30400.0 C4H8OOH1-3O2=C4H72-1OOH+HO2 2.540E+10 0.804 30098.0 C4H8OOH1-4O2=C4H71-4OOH+HO2 1.440E+07 1.380 28900.0 C4H8OOH2-3O2=C4H71-3OOH+HO2 5.130E+09 1.000 30400.0 C4H8OOH2-4O2=C4H71-3OOH+HO2 1.440E+07 1.380 28900.0 C4H8OOH1-2O2=C4H71-3,4OOH 1.440E+07 1.400 20800.0 C4H8OOH1-2O2=C4H72-3,4OOH 1.720E+09 0.900 29500.0 C4H8OOH1-2O2=NC4KET12+OH 2.440E+07 1.600 27900.0 C4H8OOH1-3O2=C4H71-2,4OOH 1.460E+09 1.100 33500.0 C4H8OOH1-3O2=C4H72-1,3OOH 1.720E+09 0.900 29500.0 C4H8OOH1-3O2=NC4KET13+OH 1.090E+04 2.400 19900.0 C4H8OOH1-4O2=C4H72-1,4OOH 1.360E+07 1.300 18200.0 DUP C4H8OOH1-4O2=C4H72-1,4OOH 4.010E+08 1.100 30100.0 DUP C4H8OOH1-4O2=NC4KET14+OH 4.800E+03 1.700 16600.0 C4H8OOH2-1O2=C4H72-3,4OOH 1.720E+09 0.900 29500.0 C4H8OOH2-1O2=C4H71-3,4OOH 1.230E+06 1.500 20000.0 C4H8OOH2-1O2=NC4KET21+OH 2.760E+08 1.200 25700.0 C4H8OOH2-3O2=C4H71-2,3OOH 1.460E+09 1.100 33500.0 DUP C4H8OOH2-3O2=C4H71-2,3OOH 1.440E+07 1.400 20800.0 DUP C4H8OOH2-3O2=NC4KET23+OH 1.750E+06 1.700 26000.0 C4H8OOH2-4O2=C4H71-2,4OOH 1.230E+06 1.500 20000.0 C4H8OOH2-4O2=C4H72-1,3OOH 4.010E+08 1.100 30100.0 C4H8OOH2-4O2=NC4KET24+OH 5.790E+01 2.900 17000.0 C4H71-3,4OOH=C4H7O1-3OOH-4+OH 2.440E+09 0.780 18000.0 C4H71-3,4OOH=C4H7O1-4OOH-2+OH 1.720E+09 0.760 11100.0 C4H72-3,4OOH=C4H7O2-3OOH-1+OH 6.990E+09 0.815 9788.0 C4H72-3,4OOH=C4H7O1-3OOH-2+OH 2.590E+09 0.690 16000.0 C4H71-2,4OOH=C4H7O1-2OOH-4+OH 2.350E+10 0.680 10800.0 C4H71-2,4OOH=C4H7O1-4OOH-2+OH 1.720E+09 0.760 11100.0 C4H72-1,3OOH=C4H7O1-2OOH-3+OH 1.710E+09 1.060 10900.0 C4H72-1,3OOH=C4H7O2-3OOH-1+OH 6.990E+09 0.815 9788.0 C4H72-1,4OOH=C4H7O1-2OOH-4+OH 1.710E+09 1.060 10900.0 C4H72-1,4OOH=C4H7O1-3OOH-4+OH 2.590E+09 0.690 16000.0 C4H71-2,3OOH=C4H7O1-2OOH-3+OH 2.350E+10 0.680 10800.0 C4H71-2,3OOH=C4H7O1-3OOH-2+OH 2.440E+09 0.780 18000.0 C4H71-3,4OOH=¿C2H4+OH+HO2CH2CHO 1.230E+09 1.300 24900.0 C4H72-3,4OOH=C4H72-1OOH+HO2 2.570E+11 0.538 15325.0 C4H71-2,4OOH=C4H71-4OOH+HO2 2.670E+11 0.500 15800.0 C4H72-1,3OOH=C4H72-1OOH+HO2 2.570E+11 0.538 15325.0 C4H72-1,3OOH=C4H71-3OOH+HO2 6.030E+09 0.950 15200.0 C4H72-1,4OOH=C4H71-4OOH+HO2 2.570E+11 0.538 15325.0 C4H71-2,3OOH=C4H71-3OOH+HO2 6.030E+09 0.950 15200.0 C4H72-1,4OOH=C4H72-1OOH+HO2 2.670E+11 0.500 15800.0 C4H72-1OOH=¿CH2O+C3H5-S+OH 1.500E+16 0.000 42000.0 C4H71-3OOH=¿C2H3CHO+CH3+OH 1.050E+16 0.000 41600.0 C4H71-3OOH=¿CH3CHO+C2H3+OH 1.050E+16 0.000 41600.0 NC4KET12=¿C2H5CHO+HCO+OH 1.050E+16 0.000 41600.0 NC4KET13=¿CH3CHO+ 1.050E+16 0.000 43000.0 NC4KET14=¿CH2CH2CHO+CH2O+OH 1.500E+16 0.000 42000.0 NC4KET21=¿CH2O

1.500E+16 0.000 42000.0 NC4KET23=¿CH3CHO+CH3CO+OH 1.050E+16 0.000 41600.0 NC4KET24=¿CH2O+C

1.500E+16 0.000 43000.0 HO2CH2CHO=¿CH2O+HCO+OH 1.500E+16 0.000 42000.0 IC4H10(+M)=CH3+IC3H7

2.520E+31 -4.102 91495.0 LOW / 2.410E+19 0.000 52576.0 / TROE / 3.662E-01 8.153E+02

6.079E+01 1.000E+20 / IC4H10=TC4H9+H 2.510E+98 -23.810 145300.0 IC4H10=IC4H9+H

9.850E+95 -23.110 147600.0 IC4H10+CH3=IC4H9+CH4 1.360E+00 3.650 7154.0 IC4H10+H=IC4H9+H2

1.810E+06 2.540 6756.0 IC4H10+OH=IC4H9+H2O 6.650E+04 2.665 -169.0 IC4H10+C2H5=IC4H9+C2H6

1.510E+12 0.000 10400.0 IC4H10+HO2=IC4H9+H2O2 6.120E+01 3.590 17160.0 IC4H10+O=IC4H9+OH

4.050E+07 2.034 5136.0 IC4H10+CH3O=IC4H9+CH3OH 4.800E+11 0.000 7000.0 IC4H10+O2=IC4H9+HO2

9.000E+13 0.000 52290.0 IC4H10+CH3O2=IC4H9+CH3O2H 2.080E+00 3.970 18280.0 IC4H10+C2H5O2=IC4H9-

2.550E+13 0.000 20460.0 IC4H10+CH3CO3=IC4H9+CH3CO3H 2.550E+13 0.000 20460.0 IC4H10+NC3H7O2=IC

2.550E+13 0.000 20460.0 IC4H10+IC3H7O2=IC4H9+IC3H7O2H 2.550E+13 0.000 20460.0 IC4H10+IC4H9O2=IC4

2.550E+13 0.000 20460.0 IC4H10+TC4H9O2=IC4H9+TC4H9O2H 2.550E+13 0.000 20460.0 IC4H10+O2CHO=IC

2.520E+13 0.000 20440.0 IC4H10+SC4H9O2=IC4H9+SC4H9O2H 2.250E+13 0.000 20460.0 IC4H10+SC4H9O2=T

2.800E+12 0.000 16000.0 IC4H10+PC4H9O2=IC4H9+PC4H9O2H 2.250E+13 0.000 20460.0 IC4H10+H=TC4H9+

6.020E+05 2.400 2583.0 IC4H10+CH3=TC4H9+CH4 9.040E-01 3.460 4598.0 IC4H10+OH=TC4H9+H2O

2.920E+04 2.531 -1659.0 IC4H10+C2H5=TC4H9+C2H6 1.000E+11 0.000 7900.0 IC4H10+HO2=TC4H9+H2O2

4.330E+02 3.010 12090.0 IC4H10+O=TC4H9+OH 1.970E+05 2.402 1150.0 IC4H10+CH3O=TC4H9+CH3OH

1.900E+10 0.000 2800.0 IC4H10+O2=TC4H9+HO2 1.000E+13 0.000 48200.0 IC4H10+O2CHO=TC4H9+HO2CH

2.800E+12 0.000 16010.0 IC4H10+PC4H9O2=TC4H9+PC4H9O2H 2.800E+12 0.000 16000.0 IC4H10+CH3O2=T

1.370E+02 3.120 13190.0 IC4H10+C2H5O2=TC4H9+C2H5O2H 2.800E+12 0.000 16000.0 IC4H10+CH3CO3=TC

2.800E+12 0.000 16000.0 IC4H10+NC3H7O2=TC4H9+NC3H7O2H 2.800E+12 0.000 16000.0 IC4H10+IC3H7O2=

2.800E+12 0.000 16000.0 IC4H10+IC4H9O2=TC4H9+IC4H9O2H 2.800E+12 0.000 16000.0 IC4H10+TC4H9O2=T

2.800E+12 0.000 16000.0 IC4H10+IC4H9=TC4H9+IC4H10 2.500E+10 0.000 7900.0 IC4H9=TC4H9

3.560E+10 0.880 34600.0 IC4H9=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-01 3.150E+41

-9.500 33486.0 / PLOG / 1.00E+00 6.750E+44 -10.070 37209.0 / PLOG / 1.00E+01 7.790E+44

-9.700 39751.0 / PLOG / 1.00E+02 3.610E+39 -7.780 39583.0 / TC4H9+HO2=TC4H9O+OH

7.000E+12 0.000 -1000.0 TC4H9+CH3O2=TC4H9O+CH3O 7.000E+12 0.000 -1000.0 TC4H9+NC3H7O2=TC4H9

7.000E+12 0.000 -1000.0 TC4H9+SC4H9O2=TC4H9O+SC4H9O 7.000E+12 0.000 -1000.0 TC4H9+PC4H9O2=T

7.000E+12 0.000 -1000.0 TC4H9+IC3H7O2=TC4H9O+IC3H7O 7.000E+12 0.000 -1000.0 IC4H9+HO2=IC4H9O+

7.000E+12 0.000 -1000.0 IC4H9+CH3O2=IC4H9O+CH3O 7.000E+12 0.000 -1000.0 IC4H9+NC3H7O2=IC4H9O+

7.000E+12 0.000 -1000.0 IC4H9+SC4H9O2=IC4H9O+SC4H9O 7.000E+12 0.000 -1000.0 IC4H9+PC4H9O2=IC4H

7.000E+12 0.000 -1000.0 IC4H9+IC3H7O2=IC4H9O+IC3H7O 7.000E+12 0.000 -1000.0 CH3COCH3+CH3=TC4H

1.500E+11 0.000 11900.0 TC4H9O+O2=IC4H8O+HO2 8.100E+11 0.000 4700.0 IC4H9O+H=IC3H7CHO+H2

1.990E+13 0.000 0.0 IC4H9O+O2=IC3H7CHO+HO2 1.930E+11 0.000 1660.0 IC4H9O+O=IC3H7CHO+OH

6.000E+12 0.000 0.0 IC4H9O+OH=IC3H7CHO+H2O 1.810E+13 0.000 0.0 IC4H9O+HO2=IC3H7CHO+H2O2

1.000E+12 0.000 0.0 IC4H9O+CH3=IC3H7CHO+CH4 2.400E+13 0.000 0.0 IC3H7CHO+H=IC4H9O

1.000E+12 0.000 5860.0 CH2O+IC3H7=IC4H9O 5.000E+10 0.000 2330.0 TC3H6CHO+H=IC3H7CHO

2.000E+14 0.000 0.0 SC4H7OH-I=IC3H7CHO 8.590E+11 0.318 55900.0 IC3H7+HCO=IC3H7CHO

1.810E+13 0.000 0.0 IC4H8O=IC3H7CHO 4.180E+13 0.000 52720.0 IC3H7CHO+HO2=IC3H7CO+H2O2

3.000E+12 0.000 11920.0 IC3H7CHO+CH3=IC3H7CO+CH4 3.980E+12 0.000 8700.0 IC3H7CHO+O=IC3H7CO+

7.180E+12 0.000 1389.0 IC3H7CHO+O2=IC3H7CO+HO2 4.000E+13 0.000 37600.0 IC3H7CHO+OH=IC3H7CO+

2.690E+10 0.760 -340.0 IC3H7CHO+H=IC3H7CO+H2 2.600E+12 0.000 2600.0 IC3H7CHO+OH=IC3H6CHO+H2

3.120E+06 2.000 -298.0 IC3H7CHO+HO2=IC3H6CHO+H2O2 2.740E+04 2.550 15500.0 IC3H7CHO+CH3O2=IC3

4.760E+04 2.550 16490.0 TC3H6CHO+H2=IC3H7CHO+H 2.160E+05 2.380 18990.0 IC3H7CHO+HO2=TC3H6C

8.000E+10 0.000 11920.0 IC3H7CHO+OH=TC3H6CHO+H2O 1.680E+12 0.000 -781.0 IC4H8O+OH=IC3H6CHO-

7.520E+04 2.490 -1474.0 IC4H8O+H=IC3H6CHO+H2 8.790E+04 2.680 2910.0 IC4H8O+HO2=IC3H6CHO+H2O2

2.450E-05 5.260 7475.0 IC4H8O+CH3O2=IC3H6CHO+CH3O2H 1.220E-05 5.260 7475.0 IC4H8O+CH3=IC3H6CH

1.990E+01 3.370 7634.0 IC4H8O+O=IC3H6CHO+OH 1.450E+05 2.470 876.0 IC4H8O+O2=IC3H6CHO+HO2

1.500E+13 0.000 50150.0 IC3H5CHO+H=TC3H6CHO 1.300E+13 0.000 1200.0 IC3H6CO+H=TC3H6CHO

1.300E+13 0.000 4800.0 IC3H6CO+OH=IC3H7+CO2 1.730E+12 0.000 -1010.0 IC3H6CO+OH=C3H6OH2-

1+CO 2.000E+12 0.000 -1010.0 TC3H6CHO+HO2=IC3H7CHO+O2 3.680E+12 0.000 1310.0 TC3H6CHO+CH3=

3.010E+12 -0.320 -131.0 TC3H6CHO+CH2O=IC3H7CHO+HCO 2.520E+08 1.900 18190.0 TC3H6CHO+IC4H8=I

4.700E+02 3.300 19840.0 TC3H6CHO+O2=TC3H6O2CHO 1.990E+17 -2.100 0.0 TC3H6O2CHO=IC3H5O2HCHO

6.000E+11 0.000 29880.0 TC3H6O2CHO=TC3H6O2HCO 1.000E+11 0.000 25750.0 IC3H5CHO+HO2=IC3H5O2H

2.230E+11 0.000 10600.0 TC3H6OCHO+OH=TC3H6CHO+HO2 2.020E+17 -1.200 21010.0 TC3H6OCHO=CH3C

3.980E+13 0.000 9700.0 TC3H6CHO+OH=IC3H6OHCHO 5.000E+13 0.000 0.0 C3H6OH2-1+HCO=IC3H6OHCHO

1.810E+13 0.000 0.0 IC3H5CHO+H=IC3H5CO+H2 7.150E+05 2.357 1577.0 IC3H5CHO+O2=IC3H5CO+HO2

2.000E+13 0.000 40700.0 IC3H5CHO+O=IC3H5CO+OH 7.180E+12 0.000 1389.0 IC3H5CHO+OH=IC3H5CO+H2

6.130E+04 2.650 -4586.0 IC3H5CHO+HO2=IC3H5CO+H2O2 1.180E-04 4.920 3684.0 IC3H5CHO+CH3=IC3H5CO

1.250E+00 3.634 4329.0 IC3H5CHO+H=IC3H4CHO-A+H2 3.640E+05 2.455 4361.0 IC3H5CHO+O2=IC3H4CHO-

A+HO2 5.960E+19 -1.670 46192.0 IC3H5CHO+OH=IC3H4CHO-A+H2O 4.460E+06 2.072 1051.0

IC3H5CHO+O=IC3H4CHO-A+OH 5.240E+11 0.700 5884.0 IC3H5CHO+HO2=IC3H4CHO-A+H2O2

3.070E-02 4.403 13547.0 IC3H5CHO+CH3=IC3H4CHO-A+CH4 2.210E+00 3.500 5675.0 IC3H5CO=C3H5-

T+CO 1.280E+20 -1.890 34460.0 C3H4-A+HCO=IC3H4CHO-A 4.020E+04 2.518 8848.0 IC3H7+CO=IC3H7CO

1.500E+11 0.000 4810.0 C2H3CHO+CH3=IC3H6CHO 1.000E+11 0.000 7800.0 SC4H7OH-I+HO2=IC3H7CHO+H

1.490E+05 1.670 6810.0 SC4H7OH-I+HOCHO=IC3H7CHO+HOCHO 2.810E-02 3.286 -4509.0

SC4H7OH-I+H=IC4H6OH+H2 7.290E+05 2.455 4361.0 SC4H7OH-I+O=IC4H6OH+OH 1.050E+12

0.700 5884.0 SC4H7OH-I+OH=IC4H6OH+H2O 4.400E+04 2.678 -827.0 SC4H7OH-I+HO2=IC4H6OH+H2O2

2.920E-01 4.120 12802.0 SC4H7OH-I+CH3=IC4H6OH+CH4 4.420E+00 3.500 5675.0 SC4H7OH-

I+CH3O=IC4H6OH+CH3OH 1.680E+11 0.000 2600.0 SC4H7OH-I+CH3O2=IC4H6OH+CH3O2H

1.930E+04 2.600 13910.0 IC4H6OH+H=¿CH3+C3H4-A+OH 4.020E+04 2.518 8848.0 TC4H9+O2=IC4H8+HO2

8.370E-01 3.590 11960.0 IC4H9+O2=IC4H8+HO2 1.070E+00 3.710 9322.0 IC4H9+O2=IC4H9O2

6.690E+13 -0.300 -187.0 TC4H9+O2=TC4H9O2 6.690E+13 -0.300 -187.0 IC4H9O2=IC4H8+HO2
1.940E+08 1.270 29600.0 IC4H9O2=IC4H8O2H-I 9.820E+07 1.300 21500.0 IC4H9O2=IC4H8O2H-
T 2.310E+09 0.800 27100.0 TC4H9O2=TC4H8O2H-I 4.520E+09 1.200 33500.0 IC4H8O2H-I=CC4H8O+OH
4.470E+11 0.000 21900.0 IC4H8O2H-I=¿OH+CH2O+C3H6 8.450E+15 -0.680 29170.0 CC4H8O+OH=¿CH2O+C3
A+H2O 5.000E+12 0.000 0.0 CC4H8O+H=¿CH2O+C3H5-A+H2 3.510E+07 2.000 5000.0 CC4H8O+O=¿CH2O+
A+OH 1.120E+14 0.000 5200.0 CC4H8O+HO2=¿CH2O+C3H5-A+H2O2 1.000E+13 0.000 15000.0
CC4H8O+CH3O2=¿CH2O+C3H5-A+CH3O2H 1.000E+13 0.000 19000.0 CC4H8O+CH3=¿CH2O+C3H5-
A+CH4 2.000E+11 0.000 10000.0 IC4H8O2H-I+O2=IC4H8OOH-IO2 9.350E+11 0.100 -1011.0
IC4H8O2H-T+O2=IC4H8OOH-TO2 5.040E+12 -0.100 -655.0 TC4H8O2H-I+O2=TC4H8OOH-IO2
2.280E+10 0.500 -786.0 IC4H8OOH-IO2=IC4KETII+OH 5.000E+10 0.000 21400.0 IC4H8OOH-
TO2=IC4KETIT+OH 4.000E+11 0.000 31500.0 IC4H8OOH-TO2=TIC4H7Q2-I 6.000E+11 0.000
34500.0 IC4H8OOH-IO2=IIC4H7Q2-I 3.750E+10 0.000 24400.0 IC4H8OOH-IO2=IIC4H7Q2-T 1.000E+11
0.000 29200.0 TC4H8OOH-IO2=TIC4H7Q2-I 9.820E+07 1.300 21500.0 IC4H8O2H-T=IC4H8O+OH
1.550E+12 0.000 13400.0 AC3H5OOH+CH2O2H=IIC4H7Q2-I 8.500E+10 0.000 10600.0 IC4H7OOH+HO2=IIC4H
T 1.000E+11 0.000 7800.0 TIC4H7Q2-I=IC4H7OOH+HO2 1.600E+12 0.230 15200.0 IC4KETII=¿CH2O+C2H5CO
1.500E+16 0.000 42000.0 IC4H9O2+CH3O2=¿IC4H9O+CH3O+O2 1.400E+16 -1.610 1860.0 IC4H9O2+C2H5O2=
1.400E+16 -1.610 1860.0 IC4H9O2+CH3CO3=¿IC4H9O+CH3CO2+O2 1.400E+16 -1.610 1860.0
IC4H9O2+IC4H9O2=¿O2+IC4H9O+IC4H9O 1.400E+16 -1.610 1860.0 IC4H9O2+TC4H9O2=¿IC4H9O+TC4H9O
1.400E+16 -1.610 1860.0 IC4H9O2+PC4H9O2=¿IC4H9O+PC4H9O+O2 1.400E+16 -1.610 1860.0
IC4H9O2+SC4H9O2=¿IC4H9O+SC4H9O+O2 1.400E+16 -1.610 1860.0 IC4H9O2+NC3H7O2=¿IC4H9O+NC3H7
1.400E+16 -1.610 1860.0 IC4H9O2+IC3H7O2=¿IC4H9O+IC3H7O+O2 1.400E+16 -1.610 1860.0
IC4H9O2+HO2=¿IC4H9O+OH+O2 1.400E+16 -1.610 1860.0 TC4H9O2+CH3O2=¿TC4H9O+CH3O+O2
1.400E+16 -1.610 1860.0 TC4H9O2+C2H5O2=¿TC4H9O+C2H5O+O2 1.400E+16 -1.610 1860.0
TC4H9O2+CH3CO3=¿TC4H9O+CH3CO2+O2 1.400E+16 -1.610 1860.0 TC4H9O2+TC4H9O2=¿O2+TC4H9O+
1.400E+16 -1.610 1860.0 TC4H9O2+PC4H9O2=¿TC4H9O+PC4H9O+O2 1.400E+16 -1.610 1860.0
TC4H9O2+SC4H9O2=¿TC4H9O+SC4H9O+O2 1.400E+16 -1.610 1860.0 TC4H9O2+NC3H7O2=¿TC4H9O+NC
1.400E+16 -1.610 1860.0 TC4H9O2+IC3H7O2=¿TC4H9O+IC3H7O+O2 1.400E+16 -1.610 1860.0
TC4H9O2+HO2=¿TC4H9O+OH+O2 1.400E+16 -1.610 1860.0 IC4H9O2+CH3=IC4H9O+CH3O
7.000E+12 0.000 -1000.0 IC4H9O2+C2H5=IC4H9O+C2H5O 7.000E+12 0.000 -1000.0 IC4H9O2+IC3H7=IC4H9O
7.000E+12 0.000 -1000.0 IC4H9O2+NC3H7=IC4H9O+NC3H7O 7.000E+12 0.000 -1000.0 IC4H9O2+PC4H9=IC4H
7.000E+12 0.000 -1000.0 IC4H9O2+SC4H9=IC4H9O+SC4H9O 7.000E+12 0.000 -1000.0 IC4H9O2+IC4H9=IC4H9
7.000E+12 0.000 -1000.0 IC4H9O2+TC4H9=IC4H9O+TC4H9O 7.000E+12 0.000 -1000.0 IC4H9O2+C3H5-
A=IC4H9O+C3H5O 7.000E+12 0.000 -1000.0 IC4H9O2+C4H71-3=IC4H9O+C4H71-O 7.000E+12
0.000 -1000.0 IC4H9O2+IC4H7=IC4H9O+IC4H7O 7.000E+12 0.000 -1000.0 TC4H9O2+CH3=TC4H9O+CH3O
7.000E+12 0.000 -1000.0 TC4H9O2+C2H5=TC4H9O+C2H5O 7.000E+12 0.000 -1000.0 TC4H9O2+IC3H7=TC4H
7.000E+12 0.000 -1000.0 TC4H9O2+NC3H7=TC4H9O+NC3H7O 7.000E+12 0.000 -1000.0 TC4H9O2+PC4H9=T

7.000E+12 0.000 -1000.0 TC4H9O2+SC4H9=TC4H9O+SC4H9O 7.000E+12 0.000 -1000.0 TC4H9O2+IC4H9=TC
7.000E+12 0.000 -1000.0 TC4H9O2+TC4H9=TC4H9O+TC4H9O 7.000E+12 0.000 -1000.0 TC4H9O2+C3H5-
A=TC4H9O+C3H5O 7.000E+12 0.000 -1000.0 TC4H9O2+C4H71-3=TC4H9O+C4H71-O 7.000E+12
0.000 -1000.0 IC4H9O2H=IC4H9O+OH 1.500E+16 0.000 42500.0 IC4H9O2+HO2=IC4H9O2H+O2
1.750E+10 0.000 -3275.0 IC4H9O2+H2O2=IC4H9O2H+HO2 2.400E+12 0.000 10000.0 IC4H9O2+H2=IC4H9O2H
3.010E+13 0.000 26030.0 IC4H9O2+CH4=IC4H9O2H+CH3 1.130E+13 0.000 20460.0 IC4H9O2+CH3OH=IC4H9O
6.300E+12 0.000 19360.0 IC4H9O2+CH2O=IC4H9O2H+HCO 1.300E+11 0.000 9000.0 IC4H9O2+C2H6=IC4H9O
1.700E+13 0.000 20460.0 IC4H9O2+C2H4=IC4H9O2H+C2H3 8.590E+00 3.754 27132.0 IC4H9O2+C2H5OH=IC4
6.300E+12 0.000 19360.0 IC4H9O2+C2H5OH=IC4H9O2H+SC2H4OH 4.200E+12 0.000 15000.0
IC4H9O2+CH3CHO=IC4H9O2H+CH3CO 2.800E+12 0.000 13600.0 IC4H9O2+C3H8=IC4H9O2H+IC3H7
2.000E+12 0.000 17000.0 IC4H9O2+C3H8=IC4H9O2H+NC3H7 1.700E+13 0.000 20460.0 IC4H9O2+C2H3CHO=
2.800E+12 0.000 13600.0 IC4H9O2+C2H5CHO=IC4H9O2H+C2H5CO 2.800E+12 0.000 13600.0
IC4H9O2+C3H6=IC4H9O2H+C3H5-A 5.350E-02 4.207 13288.0 TC4H9O2H=TC4H9O+OH 5.950E+15
0.000 42540.0 TC4H9O2+CH4=TC4H9O2H+CH3 1.130E+13 0.000 20460.0 TC4H9O2+C2H6=TC4H9O2H+C2H
1.700E+13 0.000 20460.0 TC4H9O2+C3H8=TC4H9O2H+IC3H7 2.000E+12 0.000 17000.0 TC4H9O2+C3H8=TC
1.700E+13 0.000 20460.0 TC4H9O2+CH3OH=TC4H9O2H+CH2OH 6.300E+12 0.000 19360.0
TC4H9O2+C2H5OH=TC4H9O2H+PC2H4OH 6.300E+12 0.000 19360.0 TC4H9O2+C2H5OH=TC4H9O2H+SC2
4.200E+12 0.000 15000.0 TC4H9O2+CH3CHO=TC4H9O2H+CH3CO 2.800E+12 0.000 13600.0
TC4H9O2+C2H3CHO=TC4H9O2H+C2H3CO 2.800E+12 0.000 13600.0 TC4H9O2+C2H5CHO=TC4H9O2H+C2
2.800E+12 0.000 13600.0 TC4H9O2+HO2=TC4H9O2H+O2 1.750E+10 0.000 -3275.0 TC4H9O2+H2O2=TC4H9O
2.400E+12 0.000 10000.0 TC4H9O2+CH2O=TC4H9O2H+HCO 1.300E+11 0.000 9000.0 TC4H9O2+C2H4=TC4H
8.590E+00 3.754 27132.0 TC4H9O2+H2=TC4H9O2H+H 3.010E+13 0.000 26030.0 TC4H9O2+C3H6=TC4H9O2H
A 5.350E-02 4.207 13288.0

IC4H8=IC4H7-I1+H 7.710E+69 -16.090 140000.0 IC4H8=C3H5-T+CH3 1.420E+93 -22.790
133825.0 PLOG / 1.00E-01 1.260E+94 -22.990 134024.0 / PLOG / 1.00E+00 6.760E+93 -22.510
137933.0 / PLOG / 3.50E+00 3.140E+90 -21.370 137866.0 / PLOG / 1.00E+01 9.200E+85 -19.940
136498.0 / PLOG / 3.50E+01 6.050E+78 -17.760 133437.0 / PLOG / 1.00E+02 4.870E+71 -15.650
129919.0 / IC4H8=IC4H7+H 4.660E+92 -22.450 129059.0 PLOG / 1.00E-01 7.510E+95 -23.380
129214.0 / PLOG / 1.00E+00 3.590E+88 -20.990 127813.0 / PLOG / 3.50E+00 2.960E+82 -19.120
125456.0 / PLOG / 1.00E+01 2.130E+76 -17.270 122629.0 / PLOG / 3.50E+01 1.130E+68 -14.820
118416.0 / PLOG / 1.00E+02 4.730E+60 -12.660 114404.0 / IC4H8+OH=IC4H7+H2O 4.400E+04
2.678 -827.0 IC4H8+OH=IC4H7-I1+H2O 1.090E+04 2.815 1114.0 IC4H8+O2=IC4H7+HO2 3.120E+13
0.000 37450.0 IC4H8+O2=IC4H7-I1+HO2 2.000E+13 0.000 62270.0 IC4H8+H=IC4H7+H2 7.290E+05
2.455 4361.0 IC4H8+H=IC4H7-I1+H2 8.620E+02 3.250 12167.0 IC4H8+O=IC4H7+OH 1.050E+12
0.700 5884.0 IC4H8+O=IC4H7-I1+OH 1.200E+11 0.700 8959.0 IC4H8+HO2=IC4H7+H2O2 2.920E-

01 4.120 12802.0 IC4H8+HO2=IC4H7-I1+H2O2 9.700E+04 2.549 24733.0 IC4H8+CH3=IC4H7+CH4
3.200E+12 0.000 10000.0 IC4H8+CH3=IC4H7-I1+CH4 2.000E+12 0.000 15000.0 IC4H8+CH3O=IC4H7+CH3OH
1.680E+11 0.000 2600.0 IC4H8+C3H5-A=IC4H7+C3H6 7.940E+11 0.000 20500.0 IC4H8+C3H5-
S=IC4H7+C3H6 7.940E+11 0.000 20500.0 IC4H8+C3H5-T=IC4H7+C3H6 7.940E+11 0.000 20500.0
IC4H8+CH3O2=IC4H7+CH3O2H 1.540E-01 4.403 13547.0 IC4H8+CH3CO3=IC4H7+CH3CO3H
1.540E-01 4.403 13547.0 IC4H8+O2CHO=IC4H7+HO2CHO 1.930E+04 2.600 13910.0 IC4H9O2+IC4H8=IC4H9O2
1.400E+12 0.000 14900.0 TC4H9O2+IC4H8=TC4H9O2H+IC4H7 1.400E+12 0.000 14900.0 PC4H9O2+IC4H8=PC
1.400E+12 0.000 14900.0 SC4H9O2+IC4H8=SC4H9O2H+IC4H7 1.400E+12 0.000 14900.0 IC3H7O2+IC4H8=IC3
1.400E+12 0.000 14900.0 NC3H7O2+IC4H8=NC3H7O2H+IC4H7 1.400E+12 0.000 14900.0 IC4H7O+IC4H8=IC4H
2.700E+11 0.000 4000.0 IC4H8+CH2CCH2OH=IC4H7+C3H5OH 7.940E+11 0.000 20500.0 IC4H7=IC4H7-
I1 1.300E+55 -14.530 73800.0 PLOG / 1.00E-01 1.300E+55 -14.530 73800.0 / PLOG / 1.00E+00
5.000E+51 -13.020 73300.0 / PLOG / 1.00E+01 9.700E+48 -11.730 73700.0 / PLOG / 1.00E+02
4.860E+44 -9.840 73400.0 / C3H4-A+CH3=IC4H7 4.020E+04 2.500 8848.0 IC4H7+HO2=IC4H7O+OH
1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.020E+13 -0.158 -1417.0 / PLOG / 1.00E-01 4.980E+14
-0.642 -349.0 / PLOG / 1.00E+00 7.770E+17 -1.520 2379.0 / PLOG / 1.00E+01 2.930E+15 -0.684
3615.0 / PLOG / 1.00E+02 1.640E+04 2.740 1144.0 / IC4H7+HO2=IC4H7OOH 1.000E+11 0.000
0.0 PLOG / 1.00E-02 1.910E+31 -7.230 1336.0 / PLOG / 1.00E-01 6.310E+42 -10.300 5569.0 /
PLOG / 1.00E+00 1.030E+45 -10.600 7852.0 / PLOG / 1.00E+01 2.790E+37 -7.920 6498.0 /
PLOG / 1.00E+02 1.440E+32 -6.010 6054.0 / IC4H7+HO2=IC3H5CHO+H2O 1.000E+11 0.000
0.0 PLOG / 1.00E-02 1.090E+00 3.010 -3421.0 / PLOG / 1.00E-01 6.350E+01 2.500 -2341.0
/ PLOG / 1.00E+00 6.050E+05 1.390 595.0 / PLOG / 1.00E+01 3.100E+05 1.590 2678.0 /
PLOG / 1.00E+02 5.070E-05 4.590 928.0 / IC4H7OOH=IC3H5CHO+H2O 1.000E+11 0.000 0.0
PLOG / 1.00E-02 1.990E+50 -12.700 53532.0 / PLOG / 1.00E-01 4.720E+47 -11.500 54361.0 /
PLOG / 1.00E+00 1.500E+40 -8.840 53179.0 / PLOG / 1.00E+01 2.540E+28 -5.000 49919.0 /
PLOG / 1.00E+02 1.480E+16 -1.120 45949.0 / IC4H7OOH=IC4H7O+OH 1.000E+11 0.000 0.0
PLOG / 1.00E-02 1.490E+58 -13.900 54267.0 / PLOG / 1.00E-01 1.800E+54 -12.400 54194.0 /
PLOG / 1.00E+00 3.360E+46 -9.810 52468.0 / PLOG / 1.00E+01 2.390E+36 -6.540 49429.0 /
PLOG / 1.00E+02 1.280E+27 -3.610 46333.0 / IC4H7O=C3H5-T+CH2O 1.000E+11 0.000 0.0
PLOG / 1.00E-03 7.260E+06 0.182 17816.0 / PLOG / 1.00E-02 6.970E+16 -2.500 20879.0 /
PLOG / 1.00E-01 6.640E+23 -4.230 23565.0 / PLOG / 1.00E+00 1.070E+26 -4.560 24623.0 /
PLOG / 1.00E+01 6.500E+29 -5.370 26645.0 / PLOG / 1.00E+02 4.630E+31 -5.590 28915.0
/ PLOG / 1.00E+03 8.520E+25 -3.610 27863.0 / IC4H7O=IC3H5OCH2 1.000E+11 0.000 0.0
PLOG / 1.00E-03 3.170E+20 -4.150 12121.0 / PLOG / 1.00E-02 4.790E+24 -5.030 14606.0 /
PLOG / 1.00E-01 1.900E+26 -5.160 16124.0 / PLOG / 1.00E+00 1.510E+28 -5.400 18165.0 /
PLOG / 1.00E+01 2.420E+28 -5.170 19691.0 / PLOG / 1.00E+02 5.570E+24 -3.860 19395.0 /
PLOG / 1.00E+03 1.350E+18 -1.730 17386.0 / IC4H7O=IC3H6CHO 1.000E+11 0.000 0.0 PLOG

/ 1.00E-03 5.250E-49 15.500 -15640.0 / PLOG / 1.00E-02 1.460E-88 27.600 -35995.0 / PLOG / 1.00E-01 4.440E-22 8.380 -3819.0 / PLOG / 1.00E+00 6.230E+12 -1.440 10829.0 / PLOG / 1.00E+01 3.480E+42 -9.910 25298.0 / PLOG / 1.00E+02 1.880E+38 -8.160 25974.0 / PLOG / 1.00E+03 1.670E+21 -2.740 20338.0 / IC4H7O=IC3H5CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 3.000E+15 -2.310 14668.0 / PLOG / 1.00E-02 1.500E+22 -3.960 18283.0 / PLOG / 1.00E-01 1.950E+23 -3.990 19143.0 / PLOG / 1.00E+00 1.150E+25 -4.240 20311.0 / PLOG / 1.00E+01 1.760E+28 -4.890 22765.0 / PLOG / 1.00E+02 1.410E+27 -4.280 23771.0 / PLOG / 1.00E+03 2.570E+20 -2.060 22040.0 / IC4H7O=C3H6+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 6.620E+16 -2.840 13197.0 / PLOG / 1.00E-02 1.260E+20 -3.530 15469.0 / PLOG / 1.00E-01 2.130E+21 -3.640 16584.0 / PLOG / 1.00E+00 1.070E+24 -4.160 18985.0 / PLOG / 1.00E+01 8.420E+25 -4.400 22383.0 / PLOG / 1.00E+02 1.860E+21 -2.730 23659.0 / PLOG / 1.00E+03 4.750E+08 1.140 20922.0 / IC3H5OCH2=C3H5-T+CH2O 1.000E+11 0.000 0.0 PLOG / 1.00E-03 3.300E+09 -0.638 19748.0 / PLOG / 1.00E-02 3.360E+21 -3.900 23945.0 / PLOG / 1.00E-01 2.910E+29 -5.900 27250.0 / PLOG / 1.00E+00 1.830E+34 -6.940 30690.0 / PLOG / 1.00E+01 9.720E+33 -6.500 33002.0 / PLOG / 1.00E+02 2.680E+27 -4.260 33306.0 / PLOG / 1.00E+03 8.810E+14 -0.326 31553.0 / IC3H5OCH2=IC3H6CHO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 8.010E-92 27.800 -37321.0 / PLOG / 1.00E-02 7.780E-11 3.700 -2767.0 / PLOG / 1.00E-01 5.110E+15 -2.760 15938.0 / PLOG / 1.00E+00 4.480E+25 -5.200 21532.0 / PLOG / 1.00E+01 3.970E+34 -7.410 28117.0 / PLOG / 1.00E+02 5.620E+22 -3.560 25807.0 / PLOG / 1.00E+03 2.510E+20 -2.630 29288.0 / IC3H5OCH2=IC3H5CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 4.930E+24 -5.050 20108.0 / PLOG / 1.00E-02 2.140E+28 -5.800 22219.0 / PLOG / 1.00E-01 1.930E+32 -6.640 25108.0 / PLOG / 1.00E+00 8.600E+34 -7.110 28209.0 / PLOG / 1.00E+01 2.170E+34 -6.640 30648.0 / PLOG / 1.00E+02 4.170E+28 -4.710 31232.0 / PLOG / 1.00E+03 3.980E+18 -1.620 30130.0 / IC3H5OCH2=C3H6+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 8.230E+26 -5.840 19357.0 / PLOG / 1.00E-02 1.320E+29 -6.210 21294.0 / PLOG / 1.00E-01 3.470E+32 -6.960 24197.0 / PLOG / 1.00E+00 1.440E+36 -7.760 28008.0 / PLOG / 1.00E+01 9.720E+37 -8.020 32395.0 / PLOG / 1.00E+02 2.430E+31 -5.810 34296.0 / PLOG / 1.00E+03 3.730E+14 -0.726 32008.0 / IC3H6CHO=C3H5-T+CH2O 1.000E+11 0.000 0.0 PLOG / 1.00E-03 6.890E-69 21.500 2638.0 / PLOG / 1.00E-02 5.340E-33 11.100 16749.0 / PLOG / 1.00E-01 6.110E+26 -6.010 44117.0 / PLOG / 1.00E+00 8.040E+35 -8.310 46920.0 / PLOG / 1.00E+01 5.520E+40 -9.190 50509.0 / PLOG / 1.00E+02 5.850E+35 -7.180 52038.0 / PLOG / 1.00E+03 1.930E+19 -1.940 48440.0 / IC3H6CHO=IC3H5CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 1.610E+10 -1.240 32371.0 / PLOG / 1.00E-02 5.840E+15 -2.610 32878.0 / PLOG / 1.00E-01 3.640E+23 -4.600 34275.0 / PLOG / 1.00E+00 7.580E+31 -6.630 37895.0 / PLOG / 1.00E+01 2.860E+32 -6.300 39991.0 / PLOG / 1.00E+02 1.570E+23 -3.140 38012.0 / PLOG / 1.00E+03 4.520E+12 0.214 34570.0 / IC3H6CHO=C3H6+HCO 1.000E+11 0.000 0.0 PLOG /

1.00E-03 2.900E+32 -7.240 25688.0 / PLOG / 1.00E-02 5.300E+33 -7.280 27101.0 / PLOG / 1.00E-01 2.000E+35 -7.410 29027.0 / PLOG / 1.00E+00 1.010E+34 -6.700 30018.0 / PLOG / 1.00E+01 9.760E+27 -4.630 28924.0 / PLOG / 1.00E+02 2.110E+19 -1.850 26240.0 / PLOG / 1.00E+03 1.590E+13 0.063 24086.0 / C3H5-T+CH2O=IC3H5CHO+H 1.000E+11 0.000 0.0 PLOG / 1.00E-03 2.600E+04 2.260 1510.0 / PLOG / 1.00E-02 5.130E+04 2.170 1676.0 / PLOG / 1.00E-01 3.990E+05 1.910 2218.0 / PLOG / 1.00E+00 1.750E+07 1.450 3428.0 / PLOG / 1.00E+01 1.350E+09 0.933 5173.0 / PLOG / 1.00E+02 2.240E+11 0.357 8001.0 / PLOG / 1.00E+03 6.010E+05 2.090 7896.0 / C3H5-T+CH2O=C3H6+HCO 1.000E+11 0.000 0.0 PLOG / 1.00E-03 1.110E+07 1.090 1807.0 / PLOG / 1.00E-02 2.470E+07 0.993 1995.0 / PLOG / 1.00E-01 2.470E+08 0.704 2596.0 / PLOG / 1.00E+00 1.420E+10 0.209 3934.0 / PLOG / 1.00E+01 3.450E+13 -0.726 6944.0 / PLOG / 1.00E+02 3.310E+14 -0.866 10966.0 / PLOG / 1.00E+03 1.650E+01 3.170 9400.0 / IC4H7+CH3O2=IC4H7O+CH3O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 3.330E+12 -0.158 -1417.0 / PLOG / 1.00E-01 1.660E+14 -0.642 -349.0 / PLOG / 1.00E+00 2.600E+17 -1.520 2379.0 / PLOG / 1.00E+01 9.780E+14 -0.684 3615.0 / PLOG / 1.00E+02 5.470E+03 2.740 1144.0 / IC4H7+CH3O2=IC4H7OOCH3 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.910E+31 -7.230 1336.0 / PLOG / 1.00E-01 6.310E+42 -10.300 5569.0 / PLOG / 1.00E+00 1.030E+45 -10.600 7852.0 / PLOG / 1.00E+01 2.790E+37 -7.920 6498.0 / PLOG / 1.00E+02 3.400E+29 -5.280 4540.0 / IC4H7OOCH3=IC4H7O+CH3O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 1.490E+58 -13.900 54267.0 / PLOG / 1.00E-01 1.800E+54 -12.400 54194.0 / PLOG / 1.00E+00 3.360E+46 -9.810 52468.0 / PLOG / 1.00E+01 2.390E+36 -6.540 49429.0 / PLOG / 1.00E+02 2.560E+27 -3.610 46333.0 /

IC4H7O2+IC4H7=IC4H7O+IC4H7O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 2.550E+12 -0.158 -1417.0 / PLOG / 1.00E-01 1.250E+14 -0.642 -349.0 / PLOG / 1.00E+00 1.940E+17 -1.520 2379.0 / PLOG / 1.00E+01 7.330E+14 -0.684 3615.0 / PLOG / 1.00E+02 4.100E+03 2.740 1144.0 / IC4H7O2+IC4H7=IC4H7OOIC4H7 1.000E+11 0.000 0.0 PLOG / 1.00E-02 4.780E+30 -7.230 1336.0 / PLOG / 1.00E-01 1.580E+42 -10.300 5569.0 / PLOG / 1.00E+00 2.580E+44 -10.600 7852.0 / PLOG / 1.00E+01 6.980E+36 -7.920 6498.0 / PLOG / 1.00E+02 3.600E+31 -6.010 6054.0 /

IC4H7OOIC4H7=IC4H7O+IC4H7O 1.000E+11 0.000 0.0 PLOG / 1.00E-02 3.730E+57 -13.900 54267.0 / PLOG / 1.00E-01 4.500E+53 -12.400 54194.0 / PLOG / 1.00E+00 8.400E+45 -9.810 52468.0 / PLOG / 1.00E+01 5.980E+35 -6.540 49429.0 / PLOG / 1.00E+02 3.200E+26 -3.610 46333.0 / IC4H7+NC3H7O2=IC4H7O+NC3H7O 7.000E+12 0.000 -1000.0 IC4H7+PC4H9O2=IC4H7O+PC4H9O 7.000E+12 0.000 -1000.0 IC4H7+SC4H9O2=IC4H7O+SC4H9O 7.000E+12 0.000 -1000.0 IC4H7+IC3H7O2=IC4H7 7.000E+12 0.000 -1000.0 IC4H7+TC4H9O2=IC4H7O+TC4H9O 7.000E+12 0.000 -1000.0 IC4H7+IC4H7=C3H4-A+AC5H10 9.550E+40 -9.300 12470.0 PLOG / 1.00E+00 4.100E+40 -9.300 12470.0 / PLOG /

4.00E+00 3.410E+32 -6.800 9180.0 / PLOG / 1.00E+01 1.260E+28 -5.500 7410.0 / IC4H7+IC4H7=H15DE25DM
1.000E+11 0.000 0.0 PLOG / 3.90E-02 3.270E+64 -15.935 20230.0 / PLOG / 7.80E-02 7.500E+59
-14.490 18600.0 / PLOG / 1.56E-01 1.140E+55 -12.995 16700.0 / H15DE25DM+H=H15DE25DM-
S+H2 1.420E+06 2.315 2076.0 H15DE25DM+O2=H15DE25DM-S+HO2 4.000E+14 0.000 38890.0
H15DE25DM+O=H15DE25DM-S+OH 1.590E+11 0.700 13.0 H15DE25DM+OH=H15DE25DM-
S+H2O 8.950E+04 2.637 -6.0 H15DE25DM+HO2=H15DE25DM-S+H2O2 1.000E+00 3.887 9386.0
H15DE25DM+CH3=H15DE25DM-S+CH4 1.000E+00 3.649 3374.0 H15DE25DM+H=H15DE25DM-
A+H2 7.290E+05 2.455 4361.0 H15DE25DM+O2=H15DE25DM-A+HO2 1.860E+09 1.301 40939.0
H15DE25DM+O=H15DE25DM-A+OH 1.050E+12 0.700 5884.0 H15DE25DM+OH=H15DE25DM-
A+H2O 2.530E+05 2.460 729.0 H15DE25DM+HO2=H15DE25DM-A+H2O2 2.920E-01 4.120 12802.0
H15DE25DM+CH3=H15DE25DM-A+CH4 4.420E+00 3.500 5675.0 C3H5-T+B13DE2M=H15DE25DM-
S 7.070E+03 2.480 6130.0 C3H4-A+AC5H9-D=H15DE25DM-A 2.840E+04 2.500 8848.0 H15DE25DM-
S+HO2=H15DE25DM-SO+OH 7.000E+12 0.000 -1000.0 IC3H5CHO+IC4H7=H15DE25DM-SO
2.500E+10 0.000 10530.0 C3H5-T+IC4H7CHO=H15DE25DM-SO 2.500E+10 0.000 15526.0 IC4H7CHO+OH=¿CH
A+H2O 5.060E+07 2.460 729.0 H15DE25DM-A+HO2=H15DE25DM-AO+OH 7.000E+12 0.000 -
1000.0 H15DE2M-T+CH2O=H15DE25DM-AO 2.500E+10 0.000 4787.0 IC4H7+C3H4-A=H15DE2M-
T 8.800E+03 2.480 6130.0 IC4H7-I1+H=C3H4-A+CH4 3.330E+12 0.000 0.0 IC4H7-I1+H=C3H4-
P+CH4 3.340E+12 0.000 0.0 IC4H7-I1+O=C3H6+HCO 6.000E+13 0.000 0.0 IC4H7-I1+OH=¿C3H6+HCO+H
5.000E+12 0.000 0.0 IC4H7-I1+HO2=¿C3H6+HCO+OH 2.000E+13 0.000 0.0 IC4H7-I1+HCO=IC4H8+CO
9.000E+13 0.000 0.0 IC4H7-I1+CH3=C3H4-P+C2H6 1.000E+11 0.000 0.0 IC4H7-I1+O2=CH3COCH3+HCO
3.100E+31 -5.944 5748.0 IC4H7-I1+O2=TC3H6CHO+O 5.380E+18 -2.140 5143.0 IC4H7-I1+O2=IC3H5CHO+OH
2.700E+19 -2.140 5143.0 IC4H7+O2=IC4H7O2 1.090E+10 0.567 2290.0 IC4H7+O=IC3H5CHO+H
6.030E+13 0.000 0.0 IC4H7O2=IC4H6OOH-I 1.410E+05 1.836 19820.0 IC4H7O2=CCYCCOOC-T1
1.190E+08 0.804 28020.0 IC4H7O2=C2CYCOOC-I1 1.070E+08 0.892 29720.0 IC4H7O2=IC4H7O+O
1.820E+14 0.000 60620.0 IC4H7O2=IC3H5CHO+OH 1.520E+09 1.025 39460.0 IC4H6OOH-I=CVCYCCOC+OH
6.820E+12 -0.345 42140.0 IC4H6OOH-I=C3H4-A+CH2O2H 1.180E+12 0.912 51390.0 IC4H6OOH-
I=IC3H5CHO+OH 2.420E+09 0.874 54090.0 CCYCCOOC-T1=CCYC2OCO 4.560E+11 0.927 17470.0
CCYCCOOC-T1=CCYCCOOC-I2 3.560E+13 0.000 38820.0 CCYCCOOC-I2=CHOIC3H6O 3.190E+14
0.000 3000.0 C2CYCOOC-I1=IC3H5OOCH2 4.410E+13 -0.226 18500.0 IC3H5OOCH2=CH3COCH2+CH2O
1.410E+10 0.000 1000.0 CHOIC3H6O=CH3CHCHO+CH2O 4.300E+12 0.000 9780.0 CCYC2OCO=CH3COCH2+C
1.740E+13 0.000 18150.0 C2CYCOOC-I1=CCYC2OCO 1.210E+13 0.102 20320.0 IC4H7O2+IC4H7O2=¿IC4H7O+
1.400E+16 -1.610 1860.0 IC4H7O2+IC4H8=IC4H7+IC4H7OOH 1.460E-01 4.120 12802.0 IC4H8+H=IC4H9
1.000E+00 1.000 0.0 PLOG / 1.30E-03 7.990E+81 -23.161 22239.0 / PLOG / 4.00E-02 4.240E+68
-18.427 19665.0 / PLOG / 1.00E+00 1.040E+49 -11.500 15359.0 / PLOG / 1.00E+01 6.200E+41
-8.892 14637.0 / DUP IC4H8+H=IC4H9 1.000E+00 1.000 0.0 PLOG / 1.30E-03 1.850E+26 -
5.830 3866.0 / PLOG / 4.00E-02 2.820E+30 -6.490 5471.0 / PLOG / 1.00E+00 3.780E+28 -

5.570 5625.0 / PLOG / 1.00E+01 1.460E+25 -4.280 5248.0 / PLOG / 1.00E+02 4.220E+27 -4.390 9346.0 / DUP IC4H8+H=TC4H9 1.000E+00 1.000 1.0 PLOG / 1.30E-03 1.350E+44 -10.680 8196.0 / PLOG / 4.00E-02 2.110E+57 -14.230 15147.0 / PLOG / 1.00E+00 3.260E+61 -14.940 20161.0 / PLOG / 1.00E+01 5.300E+56 -13.120 20667.0 / PLOG / 1.00E+02 1.110E+50 -10.800 20202.0 / DUP IC4H8+H=TC4H9 1.000E+00 1.000 1.0 PLOG / 1.30E-03 2.170E+130 -32.580 136140.0 / PLOG / 4.00E-02 2.250E+29 -5.840 4242.0 / PLOG / 1.00E+00 1.060E+30 -5.630 5613.0 / PLOG / 1.00E+01 6.110E+26 -4.440 5182.0 / PLOG / 1.00E+02 2.730E+23 -3.260 4597.0 / DUP IC4H8+H=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.30E-03 5.130E+08 1.350 2542.0 / PLOG / 4.00E-02 2.630E+10 0.870 3600.0 / PLOG / 1.00E+00 8.900E+11 0.470 5431.0 / PLOG / 1.00E+01 3.080E+22 -2.600 12898.0 / PLOG / 1.00E+02 4.400E+22 -2.420 16500.0 / DUP IC4H8+H=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.30E-03 7.700E+02 1.350 2542.0 / PLOG / 4.00E-02 3.940E+04 0.870 3600.0 / PLOG / 1.00E+00 1.340E+06 0.470 5431.0 / PLOG / 1.00E+01 4.130E+04 2.520 3679.0 / PLOG / 1.00E+02 8.370E+02 2.910 3981.0 / DUP IC4H8+HO2=TC4H9O2 1.040E-01 3.450 4338.0 IC4H8+HO2=IC4H8O2H-T 1.640E+04 2.430 8300.0 IC4H8+HO2=TC4H8O2H-I 1.000E+11 0.000 0.0 PLOG / 1.30E-02 6.670E+14 -2.140 14188.0 / PLOG / 9.87E-01 6.250E+06 0.640 9073.0 / PLOG / 9.87E+00 7.960E+06 0.820 8771.0 / PLOG / 9.87E+01 2.050E+13 -0.820 12919.0 / IC4H8+HO2=IC4H8O+OH 1.000E+11 0.000 0.0 PLOG / 1.30E-02 1.180E+04 2.290 11321.0 / PLOG / 9.87E-01 5.300E+04 2.100 11797.0 / PLOG / 9.87E+00 1.470E+09 0.830 14808.0 / PLOG / 9.87E+01 1.960E+17 -1.450 21195.0 / TC4H8O2H-I=IC4H8O+OH 1.000E+11 0.000 0.0 PLOG / 1.30E-02 5.230E+17 -2.970 8215.0 / PLOG / 9.87E-01 4.390E+22 -3.900 11424.0 / PLOG / 9.87E+00 4.000E+25 -4.500 13952.0 / PLOG / 9.87E+01 1.210E+27 -4.660 16324.0 / IC4H8+O=IC3H7+HCO 7.450E+06 1.880 183.0 IC4H8+O=¿CH2CO+CH3+CH3 3.050E+06 1.880 183.0 IC4H8+O=¿IC3H6CO+H+H 3.050E+06 1.880 183.0 IC4H8+OH=IC4H7OH+H 2.290E+13 0.070 10580.0 PLOG / 1.30E-03 2.670E+13 0.050 10611.0 / PLOG / 1.00E-02 2.750E+13 0.050 10623.0 / PLOG / 1.30E-02 2.870E+13 0.040 10634.0 / PLOG / 2.50E-02 1.590E+14 -0.160 11125.0 / PLOG / 1.00E-01 3.100E+14 -0.220 11407.0 / PLOG / 1.32E-01 3.780E+14 -0.240 11458.0 / PLOG / 1.00E+00 9.150E+07 1.420 10087.0 / PLOG / 1.00E+01 3.660E+05 2.140 10410.0 / PLOG / 1.00E+02 8.190E+02 2.840 10481.0 / IC4H8+OH=SC3H5OH+CH3 1.290E+06 1.650 1233.0 PLOG / 1.30E-03 5.160E+05 1.650 1233.0 / PLOG / 1.00E-02 7.280E+03 2.100 1162.0 / PLOG / 1.30E-02 8.160E+02 2.480 1128.0 / PLOG / 2.50E-02 1.150E+02 2.800 1152.0 / PLOG / 1.00E-01 5.600E+00 3.210 1208.0 / PLOG / 1.32E-01 3.080E+00 3.290 1216.0 / PLOG / 1.00E+00 4.520E+03 2.500 3238.0 / PLOG / 1.00E+01 9.640E+18 -1.740 13107.0 / PLOG / 1.00E+02 1.320E-01 3.700 3665.0 / IC4H8+OH=IC3H5OH+CH3 1.290E+06 1.650 1233.0 PLOG / 1.30E-03 2.060E+06 1.650 1233.0 / PLOG / 1.00E-02 2.910E+04 2.100 1162.0 / PLOG / 1.30E-02 3.260E+03 2.480 1128.0 / PLOG / 2.50E-02 4.610E+02 2.800 1152.0 / PLOG / 1.00E-01 2.240E+01 3.210 1208.0 / PLOG / 1.32E-

01 1.230E+01 3.290 1216.0 / PLOG / 1.00E+00 1.810E+04 2.500 3238.0 / PLOG / 1.00E+01 3.860E+19 -1.740 13107.0 / PLOG / 1.00E+02 5.280E-01 3.700 3665.0 / IC4H8+OH=SC4H7OH-I+H 2.870E+00 2.920 625.0 PLOG / 1.30E-03 2.870E+00 2.920 625.0 / PLOG / 1.00E-02 4.840E-01 2.980 704.0 / PLOG / 1.30E-02 3.130E-01 3.040 721.0 / PLOG / 2.50E-02 9.330E-03 3.620 677.0 / PLOG / 1.00E-01 4.640E-05 4.480 687.0 / PLOG / 1.32E-01 2.710E-05 4.560 707.0 / PLOG / 1.00E+00 7.650E-07 5.050 874.0 / PLOG / 1.00E+01 2.640E+15 -0.800 12728.0 / PLOG / 1.00E+02 4.870E-04 4.320 4020.0 / IC4H8+OH=CH3COCH3+CH3 6.930E+05 1.490 -536.0 PLOG / 1.30E-03 6.930E+05 1.490 -536.0 / PLOG / 1.00E-02 5.940E+03 2.010 -560.0 / PLOG / 1.30E-02 1.100E+03 2.220 -680.0 / PLOG / 2.50E-02 1.070E+02 2.500 -759.0 / PLOG / 1.00E-01 7.830E-01 3.100 -919.0 / PLOG / 1.32E-01 3.070E-01 3.220 -946.0 / PLOG / 1.00E+00 3.160E-04 4.050 -1144.0 / PLOG / 1.00E+01 7.590E-06 4.490 -680.0 / PLOG / 1.00E+02 5.450E-05 4.220 1141.0 / IC4H8+OH=IC4H8OH-IT 5.100E+54 -20.700 32402.0 PLOG / 1.30E-03 2.300E+78 -20.700 32402.0 / PLOG / 1.00E-02 2.740E+77 -20.000 33874.0 / PLOG / 1.30E-02 1.070E+76 -19.580 32874.0 / PLOG / 2.50E-02 3.680E+73 -18.790 31361.0 / PLOG / 1.00E-01 1.040E+68 -17.010 27909.0 / PLOG / 1.32E-01 7.230E+66 -16.640 27162.0 / PLOG / 1.00E+00 1.950E+59 -14.170 23079.0 / PLOG / 1.00E+01 7.580E+53 -12.230 22976.0 / PLOG / 1.00E+02 1.430E+48 -10.230 23772.0 / DUP IC4H8+OH=IC4H8OH-IT 1.420E+36 -15.840 11594.0 PLOG / 1.30E-03 6.410E+59 -15.840 11594.0 / PLOG / 1.00E-02 7.280E+59 -15.510 12898.0 / PLOG / 1.30E-02 2.790E+59 -15.340 12913.0 / PLOG / 2.50E-02 2.650E+58 -14.930 12936.0 / PLOG / 1.00E-01 1.350E+56 -14.040 12945.0 / PLOG / 1.32E-01 3.980E+55 -13.850 12887.0 / PLOG / 1.00E+00 1.550E+50 -12.040 11493.0 / PLOG / 1.00E+01 6.410E+41 -9.350 8921.0 / PLOG / 1.00E+02 2.300E+32 -6.310 6088.0 / DUP IC4H8+OH=IC4H8OH-TI 5.100E+54 -20.700 32402.0 PLOG / 1.30E-03 2.140E+59 -15.840 11594.0 / PLOG / 1.00E-02 2.430E+59 -15.510 12898.0 / PLOG / 1.30E-02 9.300E+58 -15.340 12913.0 / PLOG / 2.50E-02 8.830E+57 -14.930 12936.0 / PLOG / 1.00E-01 4.500E+55 -14.040 12945.0 / PLOG / 1.32E-01 1.330E+55 -13.850 12887.0 / PLOG / 1.00E+00 5.180E+49 -12.040 11493.0 / PLOG / 1.00E+01 2.140E+41 -9.350 8921.0 / PLOG / 1.00E+02 7.650E+31 -6.310 6088.0 / DUP IC4H8+OH=IC4H8OH-TI 1.420E+36 -15.840 11594.0 PLOG / 1.30E-03 7.680E+77 -20.700 32402.0 / PLOG / 1.00E-02 9.130E+76 -20.000 33874.0 / PLOG / 1.30E-02 3.550E+75 -19.580 32874.0 / PLOG / 2.50E-02 1.230E+73 -18.790 31361.0 / PLOG / 1.00E-01 3.450E+67 -17.010 27909.0 / PLOG / 1.32E-01 2.410E+66 -16.640 27162.0 / PLOG / 1.00E+00 6.500E+58 -14.170 23079.0 / PLOG / 1.00E+01 2.530E+53 -12.230 22976.0 / PLOG / 1.00E+02 4.780E+47 -10.230 23772.0 / DUP IC4H8OH-IT+O2=TQJC4H8OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.050E+114 -33.810 24741.0 / PLOG / 1.00E-02 2.130E+114 -33.440 26448.0 / PLOG / 1.00E-01 1.620E+110 -31.750 26612.0 / PLOG / 1.00E+00 6.000E+101 -28.790 25197.0 / PLOG / 1.00E+01 5.360E+89 -24.760 22402.0 / PLOG / 4.00E+01 1.550E+81 -21.950 20197.0 / PLOG / 1.00E+02 1.510E+75 -20.000 18578.0 / PLOG / 2.00E+02 3.160E+70

-18.480 17287.0 /

IC4H8OH-IT+O2=IC4H7OH+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.210E+26 -5.090 5755.0 / PLOG / 1.00E-02 1.410E+31 -6.550 8781.0 / PLOG / 1.00E-01 5.080E+34 -7.530 11702.0 / PLOG / 1.00E+00 1.670E+34 -7.270 13418.0 / PLOG / 1.00E+01 2.820E+28 -5.410 13318.0 / PLOG / 4.00E+01 2.500E+22 -3.520 12314.0 / PLOG / 1.00E+02 2.820E+17 -1.990 11286.0 / PLOG / 2.00E+02 1.930E+13 -0.710 10340.0 / DUP IC4H8OH-IT+O2=IC4H7OH+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 2.450E+21 -4.190 6837.0 / PLOG / 1.00E-02 1.400E+30 -6.750 11554.0 / PLOG / 1.00E-01 9.110E+39 -9.560 17834.0 / PLOG / 1.00E+00 5.160E+42 -10.170 22412.0 / PLOG / 1.00E+01 6.070E+32 -6.940 22738.0 / PLOG / 4.00E+01 3.880E+20 -3.140 20677.0 / PLOG / 1.00E+02 3.320E+10 -0.030 18552.0 / PLOG / 2.00E+02 1.220E+02 2.570 16623.0 / DUP IC4H8OH-IT+O2=SC4H7OH-I+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.260E+25 -4.690 5755.0 / PLOG / 1.00E-02 1.440E+30 -6.150 8785.0 / PLOG / 1.00E-01 4.780E+33 -7.110 11695.0 / PLOG / 1.00E+00 1.400E+33 -6.840 13395.0 / PLOG / 1.00E+01 2.120E+27 -4.960 13277.0 / PLOG / 4.00E+01 1.780E+21 -3.070 12265.0 / PLOG / 1.00E+02 1.970E+16 -1.530 11234.0 / PLOG / 2.00E+02 1.320E+12 -0.250 10285.0 / DUP IC4H8OH-IT+O2=SC4H7OH-I+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.220E+23 -4.690 5341.0 / PLOG / 1.00E-02 4.800E+28 -6.180 8461.0 / PLOG / 1.00E-01 1.710E+32 -7.160 11410.0 / PLOG / 1.00E+00 1.530E+32 -7.020 13378.0 / PLOG / 1.00E+01 5.550E+29 -6.140 15100.0 / PLOG / 4.00E+01 1.720E+26 -4.970 15849.0 / PLOG / 1.00E+02 4.460E+21 -3.510 15644.0 / PLOG / 2.00E+02 5.060E+16 -1.960 14979.0 / DUP IC4H8OH-IT+O2=TQC4H8OI 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 6.360E+104 -33.740 22390.0 / PLOG / 1.00E-02 7.960E+103 -33.010 22966.0 / PLOG / 1.00E-01 6.990E+96 -30.480 20584.0 / PLOG / 1.00E+00 1.040E+88 -27.470 16629.0 / PLOG / 1.00E+01 3.130E+96 -29.620 20346.0 / PLOG / 4.00E+01 2.790E+105 -32.040 24971.0 / PLOG / 1.00E+02 4.640E+109 -33.120 27657.0 / PLOG / 2.00E+02 2.060E+111 -33.480 29197.0 / IC4H8OH-IT+O2=¿CH3COCH3+CH2O+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.030E+37 -8.350 6940.0 / PLOG / 1.00E-02 1.070E+42 -9.640 9965.0 / PLOG / 1.00E-01 9.220E+43 -10.120 12427.0 / PLOG / 1.00E+00 1.140E+42 -9.420 13806.0 / PLOG / 1.00E+01 1.800E+38 -8.130 15131.0 / PLOG / 4.00E+01 1.610E+34 -6.800 15691.0 / PLOG / 1.00E+02 7.000E+29 -5.410 15552.0 / PLOG / 2.00E+02 3.740E+25 -4.060 15118.0 / IC4H8OH-IT+O2=QC4H7OHP 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.180E+118 -37.600 26229.0 / PLOG / 1.00E-02 1.910E+131 -40.730 34079.0 / PLOG / 1.00E-01 5.810E+138 -42.170 40750.0 / PLOG / 1.00E+00 5.050E+134 -40.190 43580.0 / PLOG / 1.00E+01 2.070E+117 -34.260 41516.0 / PLOG / 4.00E+01 1.710E+101 -29.040 38094.0 / PLOG / 1.00E+02 1.250E+89 -25.150 35203.0 / PLOG / 2.00E+02 2.980E+79 -22.090 32802.0 / IC4H8OH-IT+O2=CCY(CCO)COH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 2.110E+18 -2.870 6870.0 / PLOG / 1.00E-02

3.020E+27 -5.540 11842.0 / PLOG / 1.00E-01 1.360E+37 -8.290 18165.0 / PLOG / 1.00E+00 1.210E+39 -8.660 22517.0 / PLOG / 1.00E+01 1.530E+28 -5.130 22530.0 / PLOG / 4.00E+01 2.720E+15 -1.160 20283.0 / PLOG / 1.00E+02 1.060E+05 2.060 18044.0 / PLOG / 2.00E+02 2.300E-04 4.730 16037.0 / IC4H8OH-IT+O2=TQC4H7OHI 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.760E+53 -19.870 9019.0 / PLOG / 1.00E-02 4.680E+67 -23.920 11892.0 / PLOG / 1.00E-01 2.070E+91 -30.580 17347.0 / PLOG / 1.00E+00 2.840E+100 -32.400 20041.0 / PLOG / 1.00E+01 1.160E+115 -35.810 27656.0 / PLOG / 4.00E+01 4.870E+123 -37.830 33314.0 / PLOG / 1.00E+02 7.950E+124 -37.820 35683.0 / PLOG / 2.00E+02 4.580E+122 -36.860 36374.0 / IC4H8OH-IT+O2=C2CY(COC)OH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.420E+32 -6.950 6210.0 / PLOG / 1.00E-02 5.190E+36 -8.240 9233.0 / PLOG / 1.00E-01 5.770E+38 -8.760 11715.0 / PLOG / 1.00E+00 2.860E+36 -7.950 12823.0 / PLOG / 1.00E+01 1.370E+32 -6.510 13646.0 / PLOG / 4.00E+01 2.150E+29 -5.560 14541.0 / PLOG / 1.00E+02 1.200E+26 -4.510 14778.0 / PLOG / 2.00E+02 3.310E+22 -3.370 14606.0 / TQJC4H8OH=IC4H7OH+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 9.730E+65 -18.500 42975.0 / PLOG / 1.00E-02 1.040E+64 -17.250 44419.0 / PLOG / 1.00E-01 7.900E+59 -15.590 44504.0 / PLOG / 1.00E+00 9.350E+53 -13.490 43566.0 / PLOG / 1.00E+01 4.130E+44 -10.390 41279.0 / PLOG / 4.00E+01 6.570E+38 -8.490 39745.0 / PLOG / 1.00E+02 8.320E+34 -7.230 38675.0 / PLOG / 2.00E+02 9.460E+31 -6.280 37849.0 / DUP TQJC4H8OH=IC4H7OH+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 5.270E+64 -18.000 42872.0 / PLOG / 1.00E-02 4.820E+62 -16.740 44284.0 / PLOG / 1.00E-01 3.420E+58 -15.070 44348.0 / PLOG / 1.00E+00 4.050E+52 -12.970 43402.0 / PLOG / 1.00E+01 1.930E+43 -9.880 41120.0 / PLOG / 4.00E+01 3.280E+37 -7.990 39593.0 / PLOG / 1.00E+02 4.350E+33 -6.740 38527.0 / PLOG / 2.00E+02 5.130E+30 -5.790 37706.0 / DUP TQJC4H8OH=TQC4H8OI 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.780E+50 -12.910 31539.0 / PLOG / 1.00E-02 1.420E+45 -10.940 30864.0 / PLOG / 1.00E-01 1.500E+40 -9.210 29932.0 / PLOG / 1.00E+00 3.120E+35 -7.640 28864.0 / PLOG / 1.00E+01 2.730E+29 -5.670 27243.0 / PLOG / 4.00E+01 8.880E+25 -4.540 26272.0 / PLOG / 1.00E+02 4.600E+23 -3.800 25622.0 / PLOG / 2.00E+02 9.080E+21 -3.250 25131.0 / TQJC4H8OH=QC4H7OHP 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 9.160E+62 -18.020 45297.0 / PLOG / 1.00E-02 2.560E+62 -17.100 47393.0 / PLOG / 1.00E-01 1.250E+59 -15.610 47984.0 / PLOG / 1.00E+00 1.970E+53 -13.490 47281.0 / PLOG / 1.00E+01 1.910E+43 -10.150 44926.0 / PLOG / 4.00E+01 7.680E+36 -8.050 43267.0 / PLOG / 1.00E+02 3.490E+32 -6.640 42089.0 / PLOG / 2.00E+02 1.770E+29 -5.570 41173.0 / TQJC4H8OH=TQC4H7OHI 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 9.570E+58 -15.990 38293.0 / PLOG / 1.00E-02 7.270E+54 -14.250 38593.0 / PLOG / 1.00E-01 8.300E+49 -12.440 38031.0 / PLOG / 1.00E+00 1.900E+44 -10.510 36905.0 / PLOG / 1.00E+01 2.180E+36 -7.900 34865.0 / PLOG / 4.00E+01 4.100E+31 -6.360 33581.0 / PLOG / 1.00E+02 3.000E+28 -5.350 32704.0 / PLOG / 2.00E+02 1.340E+26 -4.590 32035.0 / TQC4H8OI=¿CH3COCH3+

1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 8.090E+38 -9.910 19096.0 / PLOG / 1.00E-02 9.090E+39 -9.930 19135.0 / PLOG / 1.00E-01 1.890E+41 -10.020 19407.0 / PLOG / 1.00E+00 7.470E+23 -4.100 14658.0 / PLOG / 1.00E+01 2.950E+33 -6.750 18685.0 / PLOG / 4.00E+01 4.240E+36 -7.560 20307.0 / PLOG / 1.00E+02 7.830E+36 -7.540 20747.0 / PLOG / 2.00E+02 7.630E+35 -7.170 20641.0 / QC4H7OHP=IC4H7OH+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.290E+57 -15.640 28576.0 / PLOG / 1.00E-02 9.650E+58 -15.750 29927.0 / PLOG / 1.00E-01 2.190E+50 -12.660 28547.0 / PLOG / 1.00E+00 1.670E+49 -12.050 29204.0 / PLOG / 1.00E+01 7.080E+40 -9.260 27188.0 / PLOG / 4.00E+01 1.320E+30 -5.820 24071.0 / PLOG / 1.00E+02 1.150E+30 -5.800 24053.0 / PLOG / 2.00E+02 1.120E+30 -5.800 24050.0 / QC4H7OHP=CCY(CCO)CO 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.110E+51 -12.970 28497.0 / PLOG / 1.00E-02 5.580E+51 -12.870 29529.0 / PLOG / 1.00E-01 3.030E+44 -10.280 28326.0 / PLOG / 1.00E+00 1.420E+44 -9.980 28986.0 / PLOG / 1.00E+01 9.690E+37 -7.930 27491.0 / PLOG / 4.00E+01 5.900E+29 -5.300 25095.0 / PLOG / 1.00E+02 5.270E+29 -5.290 25081.0 / PLOG / 2.00E+02 5.150E+29 -5.280 25078.0 / TQC4H7OHI=C2CY(COC)OH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.100E+31 -7.210 14640.0 / PLOG / 1.00E-02 1.370E+32 -7.240 14716.0 / PLOG / 1.00E-01 3.340E+33 -7.350 15127.0 / PLOG / 1.00E+00 1.860E+23 -3.680 12864.0 / PLOG / 1.00E+01 9.880E+31 -6.230 16040.0 / PLOG / 4.00E+01 1.250E+34 -6.780 17056.0 / PLOG / 1.00E+02 7.730E+33 -6.670 17176.0 / PLOG / 2.00E+02 2.130E+33 -6.450 17170.0 / TQC4H7OHI=SC4H7OH-I+HO2 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 6.010E+27 -7.270 14658.0 / PLOG / 1.00E-02 7.780E+28 -7.300 14733.0 / PLOG / 1.00E-01 3.270E+30 -7.480 15191.0 / PLOG / 1.00E+00 2.810E+17 -2.820 12336.0 / PLOG / 1.00E+01 1.920E+26 -5.220 16146.0 / PLOG / 4.00E+01 7.610E+27 -5.490 17483.0 / PLOG / 1.00E+02 1.910E+26 -4.860 17429.0 / PLOG / 2.00E+02 2.940E+24 -4.180 17285.0 /

IC4H8OH-TI+O2=IQJC4H8OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.340E+111 -32.670 25143.0 / PLOG / 1.00E-02 4.840E+107 -31.050 25460.0 / PLOG / 1.00E-01 2.410E+100 -28.420 24474.0 / PLOG / 1.00E+00 4.550E+89 -24.780 22176.0 / PLOG / 1.00E+01 1.140E+76 -20.310 18721.0 / PLOG / 4.00E+01 9.250E+66 -17.350 16238.0 / PLOG / 1.00E+02 6.200E+60 -15.360 14499.0 / PLOG / 2.00E+02 1.300E+56 -13.860 13159.0 /

IC4H8OH-TI+O2=IC3H6OHCHO+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.590E+15 -1.630 8947.0 / PLOG / 1.00E-02 5.070E+20 -3.240 11938.0 / PLOG / 1.00E-01 5.000E+25 -4.660 15251.0 / PLOG / 1.00E+00 3.180E+26 -4.790 17388.0 / PLOG / 1.00E+01 6.000E+20 -2.950 17297.0 / PLOG / 4.00E+01 1.700E+14 -0.910 16099.0 / PLOG / 1.00E+02 7.910E+08 0.730 14913.0 / PLOG / 2.00E+02 3.030E+04 2.080 13854.0 /

IC4H8OH-TI+O2=IQC4H8OT 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.120E+102 -

32.400 23496.0 / PLOG / 1.00E-02 4.230E+95 -30.040 22067.0 / PLOG / 1.00E-01 3.450E+83 -26.080 17114.0 / PLOG / 1.00E+00 8.160E+82 -25.610 16198.0 / PLOG / 1.00E+01 1.040E+97 -29.540 22648.0 / PLOG / 4.00E+01 7.250E+103 -31.420 26487.0 / PLOG / 1.00E+02 2.480E+106 -32.060 28397.0 / PLOG / 2.00E+02 1.390E+107 -32.200 29446.0 /

IC4H8OH-TI+O2=¿CH3COCH3+CH2O+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 4.390E+48 -11.880 11603.0 / PLOG / 1.00E-02 9.820E+50 -12.490 14143.0 / PLOG / 1.00E-01 3.430E+49 -11.940 15561.0 / PLOG / 1.00E+00 2.430E+45 -10.560 16415.0 / PLOG / 1.00E+01 4.980E+39 -8.680 17473.0 / PLOG / 4.00E+01 7.990E+33 -6.830 17502.0 / PLOG / 1.00E+02 1.020E+29 -5.280 17165.0 / PLOG / 2.00E+02 7.180E+24 -3.990 16747.0 /

IC4H8OH-TI+O2=CH3+C3KET21 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 2.910E+40 -9.230 10830.0 / PLOG / 1.00E-02 9.660E+43 -10.200 13698.0 / PLOG / 1.00E-01 1.340E+44 -10.130 15661.0 / PLOG / 1.00E+00 2.570E+41 -9.180 17047.0 / PLOG / 1.00E+01 1.820E+36 -7.460 18330.0 / PLOG / 4.00E+01 8.820E+29 -5.440 18205.0 / PLOG / 1.00E+02 1.740E+24 -3.650 17600.0 / PLOG / 2.00E+02 2.160E+19 -2.120 16925.0 /

IC4H8OH-TI+O2=IQC4H7OHT 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.030E+115 -35.130 25407.0 / PLOG / 1.00E-02 1.100E+129 -38.890 32891.0 / PLOG / 1.00E-01 5.150E+135 -40.380 38573.0 / PLOG / 1.00E+00 7.270E+129 -38.130 39933.0 / PLOG / 1.00E+01 4.500E+112 -32.490 37045.0 / PLOG / 4.00E+01 7.720E+97 -27.790 33612.0 / PLOG / 1.00E+02 5.170E+86 -24.260 30799.0 / PLOG / 2.00E+02 4.700E+77 -21.410 28440.0 /

IC4H8OH-TI+O2=¿IC3H5OH+CH2O+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 5.100E+24 -4.310 13009.0 / PLOG / 1.00E-02 6.910E+33 -6.970 17935.0 / PLOG / 1.00E-01 1.740E+41 -9.030 23613.0 / PLOG / 1.00E+00 2.260E+36 -7.320 25633.0 / PLOG / 1.00E+01 3.150E+17 -1.400 22782.0 / PLOG / 4.00E+01 9.350E+00 3.710 19114.0 / PLOG / 1.00E+02 5.590E-12 7.460 16156.0 / PLOG / 2.00E+02 1.270E-21 10.410 13733.0 /

IC4H8OH-TI+O2=CCY(CCOC)OH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.060E+33 -7.240 11476.0 / PLOG / 1.00E-02 6.560E+42 -9.920 17197.0 / PLOG / 1.00E-01 8.240E+46 -10.950 22090.0 / PLOG / 1.00E+00 4.480E+38 -8.220 23019.0 / PLOG / 1.00E+01 1.010E+18 -1.770 19496.0 / PLOG / 4.00E+01 1.160E+01 3.440 15637.0 / PLOG / 1.00E+02 4.850E-12 7.230 12599.0 / PLOG / 2.00E+02 8.640E-22 10.210 10126.0 / IQJC4H8OH=IC3H6OHCHO+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 3.580E+71 -20.620 52656.0 / PLOG / 1.00E-02 9.670E+71 -20.080 54935.0 / PLOG / 1.00E-01 3.390E+67 -18.180 55330.0 / PLOG / 1.00E+00 7.260E+58 -15.090 54016.0 / PLOG / 1.00E+01 4.570E+46 -11.010 51172.0 / PLOG / 4.00E+01 4.310E+38 -8.380 49054.0 / PLOG / 1.00E+02 2.120E+33 -6.660 47587.0 / PLOG / 2.00E+02

2.720E+29 -5.410 46486.0 / IQJC4H8OH=IQC4H8OT 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.040E+45 -11.200 31755.0 / PLOG / 1.00E-02 2.900E+40 -9.620 30945.0 / PLOG / 1.00E-01 4.850E+35 -8.010 29850.0 / PLOG / 1.00E+00 2.620E+30 -6.280 28498.0 / PLOG / 1.00E+01 3.370E+24 -4.370 26873.0 / PLOG / 4.00E+01 9.750E+20 -3.230 25861.0 / PLOG / 1.00E+02 5.610E+18 -2.520 25208.0 / PLOG / 2.00E+02 1.440E+17 -2.010 24740.0 /

IQJC4H8OH=IQC4H7OHT 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.360E+50 -12.930 36743.0 / PLOG / 1.00E-02 3.360E+45 -11.270 36143.0 / PLOG / 1.00E-01 1.130E+40 -9.410 34990.0 / PLOG / 1.00E+00 5.930E+33 -7.330 33438.0 / PLOG / 1.00E+01 4.240E+26 -5.000 31502.0 / PLOG / 4.00E+01 1.970E+22 -3.610 30275.0 / PLOG / 1.00E+02 3.430E+19 -2.720 29477.0 / PLOG / 2.00E+02 3.690E+17 -2.090 28900.0 /

IQC4H7OHT=¿IC3H5OH+CH2O+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 4.250E+16 -3.660 19364.0 / PLOG / 1.00E-02 2.980E+33 -8.010 27106.0 / PLOG / 1.00E-01 3.460E+38 -8.830 31412.0 / PLOG / 1.00E+00 7.070E+28 -5.460 29633.0 / PLOG / 1.00E+01 2.010E+13 -0.430 25278.0 / PLOG / 4.00E+01 1.430E+13 -0.380 25238.0 / PLOG / 1.00E+02 1.380E+13 -0.380 25234.0 / PLOG / 2.00E+02 1.370E+13 -0.370 25233.0 /

IQC4H7OHT=CCY(CCOC)OH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 1.120E+25 -5.590 19349.0 / PLOG / 1.00E-02 7.200E+32 -7.600 23093.0 / PLOG / 1.00E-01 2.220E+34 -7.650 25130.0 / PLOG / 1.00E+00 2.400E+27 -5.280 23663.0 / PLOG / 1.00E+01 2.240E+17 -2.040 20810.0 / PLOG / 4.00E+01 1.820E+17 -2.010 20786.0 / PLOG / 1.00E+02 1.780E+17 -2.010 20783.0 / PLOG / 2.00E+02 1.770E+17 -2.010 20782.0 /

IQC4H7OHT=IC4H7OOH+OH 1.420E+36 -15.840 11594.0 PLOG / 1.00E-03 6.070E+13 -4.210 22478.0 / PLOG / 1.00E-02 9.740E+39 -10.890 33616.0 / PLOG / 1.00E-01 2.180E+49 -12.650 40359.0 / PLOG / 1.00E+00 3.320E+37 -8.420 38539.0 / PLOG / 1.00E+01 2.340E+16 -1.560 32712.0 / PLOG / 4.00E+01 1.440E+16 -1.490 32656.0 / PLOG / 1.00E+02 1.380E+16 -1.480 32651.0 / PLOG / 2.00E+02 1.370E+16 -1.480 32649.0 / IQC4H8OT=¿CH3COCH3+CH2O+OH 3.640E+09 1.300 23700.0 IQC4H8OT=CH3+C3KET21 4.950E+10 0.830 27900.0 IQC4H7OHT=CH2COHCH2OOH 4.950E+10 0.830 27900.0 TQC4H7OHIO2=TQC4H7OHIQ-I 2.560E+12 -0.130 34360.0 TQC4H7OHIQ-I=¿HO2CHO+CH3COCH3+OH 5.820E+05 2.400 22790.0 TQC4H7OHIQ-I=IC4KETIT+HO2 1.830E+10 0.790 15100.0 IC4KETIT=¿CH3COCH3+HCO+OH 9.500E+15 0.000 42540.0 IC4KETIT+OH=TC3H6O2HCO+H 6.130E+04 2.654 -4586.0 IC4KETIT+HO2=TC3H6O2HCO+H2O2 1.180E-04 4.920 3684.0 TC3H6O2HCO=¿CH3C 1.280E+20 -1.890 34460.0 TQC4H7OHIO2=TQC4H7OHIQ-P 5.690E+08 0.780 21850.0 TQC4H7OHIQ-P=IC3H5COHQ+HO2 1.830E+10 0.790 15100.0 TQC4H7OHIQ-P=CH2CQCOHQ+CH3 5.380E+11 0.070 24800.0 TQC4H7OHIQ-P=¿IC3H5Q+HOCHO+OH 5.380E+11 0.070 24800.0 TQC4H7OHIQ-P=COHQCYC(COC)+OH 2.280E+08 1.290 9890.0 TQC4H7OHIQ-P=QCYC(CCOC)OH+OH 4.580E+15

-1.080 18440.0 IC3H5COHQ=¿HOCHO+C3H5-T+OH 1.590E+20 -1.500 42879.0 CH2CQCOHQ=¿HOCHO+CH2C
1.590E+20 -1.500 42879.0 CH2CQCOHQ=¿HCO+CH2CO+3OH 1.590E+20 -1.500 42879.0 IC3H5Q=¿CH2CO+C
1.590E+20 -1.500 42879.0 COHQCYC(COC)=¿HOCHO+CH2O+C2H3+OH 1.590E+20 -1.500 42879.0
QCYC(CCOC)OH=¿HOCHO+CH2CO+CH3+OH 1.590E+20 -1.500 42879.0 TQC4H7OHIO2=TQC4H7OHTO2
2.960E+09 0.040 16350.0 TQC4H7OHTO2=HOCOCQ(CH3)2+OH 1.750E+08 1.700 26000.0 HO-
COCQ(CH3)2=¿CO+CH3COCH3+2OH 1.590E+20 -1.500 42879.0 IQC4H7OHTO2=IQC4H7OHTQ-
P 2.060E+07 1.000 21070.0 IQC4H7OHTQ-P=¿OH+CH2O+CH2COHCH2OOH 1.200E+10 0.350
15700.0 CH2COHCH2OOH=¿OH+CH2O+CH2CO+H 1.590E+20 -1.500 42879.0 IQC4H7OHTQ-
P=OH+IC4H6Q2-II 1.000E+11 0.000 0.0 PLOG / 1.00E-02 2.530E+40 -9.910 32631.0 / PLOG
/ 1.00E-01 2.540E+37 -8.720 32910.0 / PLOG / 1.00E+00 1.120E+31 -6.530 31807.0 / PLOG /
1.00E+01 1.980E+21 -3.340 29138.0 / PLOG / 1.00E+02 1.950E+10 0.154 25612.0 / IC4H6Q2-
II=¿OH+CH2O+HO2+C3H4-A 1.590E+20 -1.500 42879.0 IQC4H7OHTO2=IQC4H8OTQ-I 4.130E+07
1.000 21070.0 IQC4H8OTQ-I=¿OH+CH2O+C3KET21 1.200E+10 0.350 15700.0 IQC4H8OTQ-
I=CH3+CO(CH2OOH)2 2.740E+13 0.240 29830.0 CO(CH2OOH)2=¿2OH+2CH2O+CO 1.590E+20
-1.500 42879.0 IQC4H7OHTO2=CHOC(CH3)OHCH2Q+OH 1.200E+10 0.350 15700.0 CHOC(CH3)OHCH2Q=¿OH
1.590E+20 -1.500 42879.0 C3Y12+OH=¿2CO+CH3+H2O 6.130E+04 2.654 -4586.0 TQC4H7OHI+O2=TQC4H7O
3.490E+14 -0.816 -536.0 IQC4H7OHT+O2=IQC4H7OHTO2 6.870E+16 -1.627 199.0 C2CY(COC)OH+OH=¿IC3H
2.260E+03 2.730 -4688.0 C2CY(COC)OH+HO2=¿IC3H6CO+OH+H2O2 8.600E+00 3.460 9732.0
CCY(CCO)COH+OH=¿IC3H5CHO+OH+H2O 5.660E+02 2.930 -4039.0 CCY(CCO)COH+HO2=¿IC3H5CHO+OH
1.810E-01 3.980 9057.0 CCY(CCO)COH+OH=¿PC3H4OH-2+CH2O+H2O 1.260E+03 2.970 -2661.0
CCY(CCO)COH+HO2=¿PC3H4OH-2+CH2O+H2O2 1.400E-05 5.260 8268.0 CCY(CCOC)OH+OH=¿CH2O+SC3
5.660E+02 2.930 -4039.0 CCY(CCOC)OH+HO2=¿CH2O+SC3H4OH+H2O2 1.810E-01 3.980 9057.0
IC4H7+OH=IC4H7OH 3.000E+13 0.000 0.0 IC4H7O+H=IC4H7OH 4.000E+13 0.000 0.0 IC4H6OH+H=IC4H7OH
1.000E+14 0.000 0.0 CH2CCH2OH+CH3=IC4H7OH 3.000E+13 0.000 0.0 IC4H7OH+O2=IC4H6OH+HO2
6.000E+13 0.000 39900.0 IC4H7OH+OH=IC4H6OH+H2O 1.260E+03 2.970 -2661.0 IC4H7OH+HO2=IC4H6OH+
1.450E-05 5.260 8268.0 IC4H6OH+H2=IC4H7OH+H 2.160E+04 2.380 18990.0 IC4H6OH+CH2O=IC4H7OH+HCO
6.300E+08 1.900 18190.0 IC4H6OH+IC4H8=IC4H7OH+IC4H7 4.700E+02 3.300 19840.0 IC4H7O+H2=IC4H7OH
9.050E+06 2.000 17830.0 IC4H7OH+HCO=IC4H7O+CH2O 3.020E+11 0.000 18160.0 C3H4-A+CH2OH=IC4H6O
1.000E+11 0.000 9200.0 IC4H7O=IC4H6OH 1.390E+11 0.000 15600.0 IC4H6OH+HO2=¿CH2CCH2OH+CH2O+O
1.450E+13 0.000 0.0 IC4H7OH+H=IC4H8OH 1.000E+13 0.000 1200.0 IC4H7O+O2=IC3H5CHO+HO2
3.000E+10 0.000 1649.0 IC4H7O+HO2=IC3H5CHO+H2O2 3.000E+11 0.000 0.0 IC4H7O+CH3=IC3H5CHO+CH4
2.400E+13 0.000 0.0 IC4H7O+O=IC3H5CHO+OH 6.000E+12 0.000 0.0 IC4H7O+OH=IC3H5CHO+H2O
1.810E+13 0.000 0.0 IC4H7O+H=IC3H5CHO+H2 1.990E+13 0.000 0.0 IC3H6OHCHO+OH=¿TC3H6OH+CO+H2
6.130E+04 2.650 -4586.0 IC3H6OHCHO+H=¿TC3H6OH+CO+H2 8.660E+05 2.300 1426.0 IC3H6OHCHO+HO2=
1.010E-04 5.000 3429.0 IC3H6OHCHO+CH3=¿TC3H6OH+CO+CH4 3.940E+00 3.600 4223.0 TC3H6OH=CH3CO
8.980E+11 0.271 32990.0 TC3H6OH=IC3H5OH+H 4.210E+10 1.005 40900.0 TC3H6OH+O2=CH3COCH3+HO2

2.230E+13 0.000 0.0 C3H5-A+CH3(+M)=C4H8-1(+M) 1.000E+14 -0.320 -262.0 LOW / 3.910E+60 -12.810 6250.0 / TROE / 1.040E-01 1.606E+03 6.000E+04 6.118E+03 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ C2H5+C2H3(+M)=C4H8-1(+M) 1.500E+13 0.000 0.0 LOW / 1.550E+56 -11.790 8984.0 / TROE / 1.980E-01 2.278E+03 6.000E+04 5.723E+03 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ C4H71-4+H(+M)=C4H8-1(+M) 3.600E+13 0.000 0.0 LOW / 3.010E+48 -9.320 5834.0 / TROE / 4.980E-01 1.314E+03 1.314E+03 5.000E+04 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ C4H71-3+H=C4H8-1 5.000E+13 0.000 5000.0 C3H5-S+CH3(+M)=C4H8-2(+M) 5.000E+13 0.000 0.0 LOW / 8.540E+58 -11.940 9770.0 / TROE / 1.750E-01 1.341E+03 6.000E+04 1.014E+04 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/C2H2/3.00/ C2H4/3.00/ C4H8-2=C3H5-A+CH3 7.500E+65 -15.600 97300.0 C4H8-2=H+C4H71-3 4.600E+84 -20.030 132787.0 C4H8-1+OH=C4H71-3+H2O 7.770E+05 2.200 -437.0 C4H8-1+OH=C4H71-4+H2O 8.600E+06 2.030 2623.0 C4H8-1+OH=C4H71-2+H2O 3.000E+06 1.970 2848.0 C4H8-1+OH=C4H71-1+H2O 6.930E+06 1.920 4962.0 C4H8-2+OH=C4H71-3+H2O 4.460E+06 2.072 1051.0 C4H8-2+OH=C4H72-2+H2O 6.000E+06 1.970 2846.0 C4H8-1+HO2=C4H71-3+H2O2 7.820E-01 3.970 11702.0 C4H8-2+HO2=C4H71-3+H2O2 6.900E-01 4.000 12103.0 C4H8-1+HO2=C4H71-4+H2O2 4.080E+01 3.590 17160.0 C4H8-1+HO2=C4H71-1+H2O2 9.570E+02 3.059 20799.0 C4H8-1+HO2=C4H71-2+H2O2 1.560E+04 2.820 24428.0 C4H8-2+HO2=C4H72-2+H2O2 3.120E+04 2.820 24428.0 C4H8-1+H=C4H71-4+H2 3.840E+04 2.870 6611.0 C4H8-1+H=C4H71-3+H2 2.420E+03 3.050 1995.0 C4H8-1+H=C4H71-2+H2 2.370E+04 2.850 8917.0 C4H8-1+H=C4H71-1+H2 2.630E+04 2.830 12050.0 DUP C4H8-1+H=C4H71-1+H2 2.230E+04 2.850 11710.0 DUP C4H8-2+H=C4H71-3+H2 5.620E+02 3.500 1627.0 C4H8-2+H=C4H72-2+H2 8.470E+04 2.760 9304.0 C4H8-1+O=C4H71-3+OH 1.750E+11 0.700 5884.0 C4H8-2+O=C4H71-3+OH 2.190E+11 0.810 7550.0 C4H8-1+O=C4H71-1+OH 1.200E+11 0.700 8959.0 C4H8-1+O=C4H71-2+OH 6.030E+10 0.700 7632.0 C4H8-2+O=C4H72-2+OH 1.210E+11 0.700 7632.0 C4H8-1+O=C4H71-4+OH 1.130E+14 0.000 7850.0 C4H8-1+O2=C4H71-3+HO2 1.000E+14 0.000 37190.0 !C4H8-1+O2=C4H71-3+HO2 4.880E+01 3.480 34800.0 C4H8-2+O2=C4H71-3+HO2 2.000E+14 0.000 39390.0 !C4H8-2+O2=C4H71-3+HO2 7.740E+14 3.520 36900.0 C4H8-1+O2=C4H71-1+HO2 2.000E+13 0.000 62270.0 C4H8-1+O2=C4H71-2+HO2 1.000E+13 0.000 58770.0 C4H8-2+O2=C4H72-2+HO2 2.000E+13 0.000 58770.0 C4H8-1+O2=C4H71-4+HO2 6.000E+13 0.000 52340.0 C4H8-1+CH3=C4H71-3+CH4 2.210E+00 3.500 5675.0 C4H8-1+CH3=C4H71-4+CH4 4.520E-01 3.650 7154.0 C4H8-2+CH3=C4H71-3+CH4 7.140E+00 3.570 7642.0 C4H8-1+CH3=C4H71-1+CH4 1.350E+00 3.500 12850.0 C4H8-1+CH3=C4H71-2+CH4 8.400E-01 3.500 11660.0 C4H8-2+CH3=C4H72-2+CH4 1.680E+00 3.500 11660.0 C4H8-1+CH3O2=C4H71-3+CH3O2H 2.700E+04 0.700 5884.0 C4H8-1+CH3O2=C4H71-4+CH3O2H 2.380E+03 2.550 16490.0 C4H8-1+CH3O=C4H71-3+CH3OH 4.000E+01 2.900 8609.0 C4H8-1+CH3O=C4H71-4+CH3OH 2.170E+11 0.000 6458.0 C4H8-2+CH3O=C4H71-3+CH3OH 1.800E+01 2.950 11990.0 C4H8-1+CH3CO3=C4H71-3+CH3CO3H 1.000E+11 0.000 8000.0 C4H8-

1+C3H5-A=C4H71-3+C3H6 7.900E+10 0.000 12400.0 C4H8-1+C2H5O2=C4H71-3+C2H5O2H 1.400E+12 0.000 14900.0 C4H8-1+NC3H7O2=C4H71-3+NC3H7O2H 1.400E+12 0.000 14900.0 C4H8-1+IC3H7O2=C4H71-3+IC3H7O2H 1.400E+12 0.000 14900.0 C4H8-1+PC4H9O2=C4H71-3+PC4H9O2H 1.400E+12 0.000 14900.0 C4H8-1+SC4H9O2=C4H71-3+SC4H9O2H 1.400E+12 0.000 14900.0 C4H8-2+NC3H7O2=C4H71-3+NC3H7O2H 3.200E+12 0.000 14900.0 C4H8-2+IC3H7O2=C4H71-3+IC3H7O2H 3.200E+12 0.000 14900.0 C4H8-2+PC4H9O2=C4H71-3+PC4H9O2H 3.200E+12 0.000 14900.0 C4H8-2+SC4H9O2=C4H71-3+SC4H9O2H 3.200E+12 0.000 14900.0 C4H71-3+C2H5=C4H8-1+C2H4 2.590E+12 0.000 -131.0 C4H71-3+CH3O=C4H8-1+CH2O 2.410E+13 0.000 0.0 IC4H9O2+C4H8-1=IC4H9O2H+C4H71-3 1.400E+12 0.000 14900.0 TC4H9O2+C4H8-1=TC4H9O2H+C4H71-3 1.400E+12 0.000 14900.0 IC4H9O2+C4H8-2=IC4H9O2H+C4H71-3 1.400E+12 0.000 14900.0 TC4H9O2+C4H8-2=TC4H9O2H+C4H71-3 1.400E+12 0.000 14900.0 C4H71-1=C4H6-1+H 8.950E+08 1.140 35636.0 C4H71-1=C2H5+C2H2 2.850E+12 0.680 33178.0 C4H71-2=C4H6-1+H 9.790E+08 1.200 38081.0 C4H71-2=C4H612+H 1.990E+08 1.560 37683.0 C4H71-2=C3H4-A+CH3 1.230E+10 1.190 32916.0 C4H71-3=C4H612+H 3.950E+11 0.930 61611.0 C4H71-3=C4H6+H 8.530E+07 1.950 47490.0 C4H71-4=C2H4+C2H3 2.840E+10 0.990 38999.0 C4H71-4=C4H6+H 1.320E+05 2.280 33246.0 C4H72-2=C4H6-2+H 7.870E+09 1.160 36173.0 C4H72-2=C4H612+H 9.540E+07 1.810 38993.0 C4H72-2=C3H4-P+CH3 6.300E+11 0.930 34754.0 C4H71-3=C4H71-4 5.620E-12 7.190 36201.0 C4H71-3=C4H72-2 6.760E-23 10.210 41574.0 C4H71-3+HO2=C4H71-3OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01 1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06 0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13 -1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15 -1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17 -2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18 -2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19 -2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / C4H71-3+HO2=C4H71-O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C4H71-3+HO2=C2H3COCH3+H2O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 5.160E+14 -1.740 1910.0 / PLOG / 1.00E-01 1.620E+16 -2.160 3167.0 / PLOG / 1.00E+00 9.730E+20 -3.470 7339.0 / PLOG / 2.00E+00 1.700E+23 -4.090 9378.0 / PLOG / 5.00E+00 4.330E+26 -5.020 12574.0 / PLOG / 1.00E+01 2.590E+29 -5.780 15275.0 / PLOG / 3.00E+01 7.850E+33 -7.010 19801.0 / PLOG / 5.00E+01 8.840E+35 -7.580 21918.0 / C4H71-3OOH=C4H71-O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 4.410E+35 -7.370 39745.0 / PLOG / 1.00E-01 6.640E+37 -7.600 44224.0 / PLOG / 1.00E+00 7.090E+37 -7.240 47692.0 / PLOG / 2.00E+00 1.920E+37 -6.970 48350.0 / PLOG / 5.00E+00 1.200E+36 -6.510 48849.0 / PLOG / 1.00E+01 7.170E+34 -6.080 48933.0 / PLOG / 3.00E+01 3.690E+32 -5.320 48614.0 / PLOG / 5.00E+01 3.040E+31 -4.970 48341.0 / C4H71-3OOH=C2H3COCH3+H2O 1.000E+00 1.000 1.0

PLOG / 1.00E-02 3.580E+23 -4.640 38121.0 / PLOG / 1.00E-01 2.850E+27 -5.360 43407.0 / PLOG / 1.00E+00 2.630E+29 -5.530 48042.0 / PLOG / 2.00E+00 2.830E+29 -5.430 49101.0 / PLOG / 5.00E+00 1.040E+29 -5.180 50137.0 / PLOG / 1.00E+01 2.120E+28 -4.890 50610.0 / PLOG / 3.00E+01 5.390E+26 -4.330 50818.0 / PLOG / 5.00E+01 7.760E+25 -4.040 50737.0 / C4H71-O=C2H3+CH3CHO 8.520E+25 -3.610 27863.0 C4H71-O=AC3H5OCH2 1.350E+18 -1.730 17386.0 C4H71-O=CH2CH2COCH3 1.670E+21 -2.740 20338.0 C4H71-O=C2H3COCH3+H 2.570E+20 -2.060 22040.0 C4H71-O=C2H4+CH3CO 4.750E+08 1.140 20922.0 AC3H5OCH2=C3H5-A+CH2O 8.810E+14 -0.326 31553.0 AC3H5OCH2=CH2CH2COCH3 2.510E+20 -2.630 29288.0 AC3H5OCH2=C2H3COCH3- 3.980E+18 -1.620 30130.0 AC3H5OCH2=C3H6+HCO 3.730E+14 -0.726 32008.0 CH2CH2COCH3=C2H3+CH3CH 1.930E+19 -1.940 48440.0 CH2CH2COCH3=C2H3COCH3+H 4.520E+12 0.214 34570.0 CH2CH2COCH3=C2H4+C 1.590E+13 0.063 24086.0 C2H3+CH3CHO=C2H4+CH3CO 1.650E+01 3.170 9400.0 C4H71-3+HO2=C4H72-1OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.000E+07 -0.330 -17896.0 / PLOG / 1.00E-01 1.150E+11 -1.160 -14831.0 / PLOG / 1.00E+00 2.950E+16 -2.330 -9451.0 / PLOG / 2.00E+00 7.680E+17 -2.620 -7705.0 / PLOG / 5.00E+00 2.210E+19 -2.890 -5556.0 / PLOG / 1.00E+01 1.140E+20 -2.990 -4159.0 / PLOG / 3.00E+01 2.800E+20 -2.960 -2503.0 / PLOG / 5.00E+01 2.400E+20 -2.880 -1971.0 / C4H71-3+HO2=C4H7O2-1+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.810E+20 -2.680 217.0 / PLOG / 1.00E-01 2.250E+22 -3.100 1516.0 / PLOG / 1.00E+00 2.750E+27 -4.490 6067.0 / PLOG / 2.00E+00 6.270E+29 -5.140 8273.0 / PLOG / 5.00E+00 1.960E+33 -6.090 11661.0 / PLOG / 1.00E+01 1.160E+36 -6.850 14456.0 / PLOG / 3.00E+01 2.510E+40 -8.040 19009.0 / PLOG / 5.00E+01 2.180E+42 -8.580 21090.0 / C4H71-3+HO2=SC3H5CHO+H2O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.620E+14 -1.600 1519.0 / PLOG / 1.00E-01 3.190E+15 -1.960 2620.0 / PLOG / 1.00E+00 1.690E+20 -3.260 6800.0 / PLOG / 2.00E+00 3.390E+22 -3.890 8918.0 / PLOG / 5.00E+00 1.090E+26 -4.850 12249.0 / PLOG / 1.00E+01 7.810E+28 -5.630 15058.0 / PLOG / 3.00E+01 3.140E+33 -6.890 19743.0 / PLOG / 5.00E+01 4.070E+35 -7.480 21927.0 / C4H72-1OOH=C4H7O2-1+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 5.070E+35 -7.390 39733.0 / PLOG / 1.00E-01 7.690E+37 -7.630 43994.0 / PLOG / 1.00E+00 2.760E+37 -7.140 47024.0 / PLOG / 2.00E+00 4.320E+36 -6.810 47507.0 / PLOG / 5.00E+00 1.210E+35 -6.240 47760.0 / PLOG / 1.00E+01 3.920E+33 -5.740 47658.0 / PLOG / 3.00E+01 8.620E+30 -4.880 47084.0 / PLOG / 5.00E+01 5.290E+29 -4.500 46721.0 / C4H72-1OOH=SC3H5CHO+H2O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.150E+24 -4.780 38584.0 / PLOG / 1.00E-01 9.650E+27 -5.510 43561.0 / PLOG / 1.00E+00 2.330E+29 -5.530 47626.0 / PLOG / 2.00E+00 1.290E+29 -5.350 48469.0 / PLOG / 5.00E+00 1.810E+28 -4.980 49208.0 / PLOG / 1.00E+01 1.760E+27 -4.610 49458.0 / PLOG / 3.00E+01 1.590E+25 -3.910 49357.0 / PLOG / 5.00E+01 1.580E+24 -3.580 49164.0 / C4H7O2-1=C3H5-S+CH2O 8.520E+25 -3.610 27863.0 C4H7O2-1=SC3H5OCH2-1 1.350E+18 -1.730 17386.0 C4H7O2-1=C3H6CHO-2 1.670E+21 -2.740 20338.0 C4H7O2-1=SC3H5CHO+H 2.570E+20 -2.060 22040.0 C4H7O2-1=C3H6+HCO 4.750E+08 1.140 20922.0 SC3H5OCH2-1=C3H5-

S+CH2O 8.810E+14 -0.326 31553.0 SC3H5OCH2-1=C3H6CHO-2 2.510E+20 -2.630 29288.0 SC3H5OCH2-1=SC3H5CHO+H 3.980E+18 -1.620 30130.0 SC3H5OCH2-1=C3H6+HCO 3.730E+14 -0.726 32008.0 C3H6CHO-2=C3H5-S+CH2O 1.930E+19 -1.940 48440.0 C3H6CHO-2=SC3H5CHO+H 4.520E+12 0.214 34570.0 C3H6CHO-2=C3H6+HCO 1.590E+13 0.063 24086.0 C3H5-S+CH2O=C3H6+HCO 1.650E+01 3.170 9400.0 C4H71-3+CH3O2=C4H71-3OOCH3 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.030E+01 1.240 -22589.0 / PLOG / 1.00E-01 1.850E+06 0.080 -18331.0 / PLOG / 1.00E+00 1.010E+13 -1.450 -11709.0 / PLOG / 2.00E+00 7.450E+14 -1.870 -9604.0 / PLOG / 5.00E+00 9.250E+16 -2.310 -6991.0 / PLOG / 1.00E+01 1.440E+18 -2.550 -5260.0 / PLOG / 3.00E+01 1.730E+19 -2.710 -3140.0 / PLOG / 5.00E+01 2.670E+19 -2.700 -2438.0 / C4H71-3+CH3O2=C4H71-O+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 3.450E+20 -2.680 229.0 / PLOG / 1.00E-01 2.250E+22 -3.180 1760.0 / PLOG / 1.00E+00 4.310E+27 -4.630 6415.0 / PLOG / 2.00E+00 9.600E+29 -5.280 8578.0 / PLOG / 5.00E+00 2.730E+33 -6.220 11879.0 / PLOG / 1.00E+01 1.490E+36 -6.970 14600.0 / PLOG / 3.00E+01 2.790E+40 -8.140 19040.0 / PLOG / 5.00E+01 2.220E+42 -8.670 21071.0 / C4H71-3OOCH3=C4H71-O+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.210E+35 -7.370 39745.0 / PLOG / 1.00E-01 3.320E+37 -7.600 44224.0 / PLOG / 1.00E+00 3.550E+37 -7.240 47692.0 / PLOG / 2.00E+00 9.600E+36 -6.970 48350.0 / PLOG / 5.00E+00 6.000E+35 -6.510 48849.0 / PLOG / 1.00E+01 3.590E+34 -6.080 48933.0 / PLOG / 3.00E+01 1.850E+32 -5.320 48614.0 / PLOG / 5.00E+01 1.520E+31 -4.970 48341.0 / C4H71-3+CH3O2=C4H72-1OOCH3 1.000E+00 1.000 1.0 PLOG / 1.00E-02 5.000E+06 -0.330 -17896.0 / PLOG / 1.00E-01 5.750E+10 -1.160 -14831.0 / PLOG / 1.00E+00 1.480E+16 -2.330 -9451.0 / PLOG / 2.00E+00 3.840E+17 -2.620 -7705.0 / PLOG / 5.00E+00 1.110E+19 -2.890 -5556.0 / PLOG / 1.00E+01 5.700E+19 -2.990 -4159.0 / PLOG / 3.00E+01 1.400E+20 -2.960 -2503.0 / PLOG / 5.00E+01 1.200E+20 -2.880 -1971.0 / C4H71-3+CH3O2=C4H7O2-1+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 3.410E+20 -2.680 217.0 / PLOG / 1.00E-01 1.130E+22 -3.100 1516.0 / PLOG / 1.00E+00 1.380E+27 -4.490 6067.0 / PLOG / 2.00E+00 3.140E+29 -5.140 8273.0 / PLOG / 5.00E+00 9.800E+32 -6.090 11661.0 / PLOG / 1.00E+01 5.800E+35 -6.850 14456.0 / PLOG / 3.00E+01 1.260E+40 -8.040 19009.0 / PLOG / 5.00E+01 1.090E+42 -8.580 21090.0 / C4H72-1OOCH3=C4H7O2-1+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.540E+35 -7.390 39733.0 / PLOG / 1.00E-01 3.850E+37 -7.630 43994.0 / PLOG / 1.00E+00 1.380E+37 -7.140 47024.0 / PLOG / 2.00E+00 2.160E+36 -6.810 47507.0 / PLOG / 5.00E+00 6.050E+34 -6.240 47760.0 / PLOG / 1.00E+01 1.960E+33 -5.740 47658.0 / PLOG / 3.00E+01 4.310E+30 -4.880 47084.0 / PLOG / 5.00E+01 2.650E+29 -4.500 46721.0 / C4H71-3+C2H5O2=C4H71-O+C2H5O 3.800E+12 0.000 -1200.0 IC3H7O2+C4H71-3=IC3H7O+C4H71-O 3.800E+12 0.000 -1200.0 NC3H7O2+C4H71-3=NC3H7O+C4H71-O 3.800E+12 0.000 -1200.0 C4H71-O=C2H3CHO+CH3 7.940E+14 0.000 19000.0 C4H71-3+O=C2H3CHO+CH3 6.030E+13 0.000 0.0 C4H71-3+O2=C4H6+HO2 1.070E+00 3.710 9322.0 H+C4H71-3=C4H6+H2 3.160E+13 0.000 0.0 C2H5+C4H71-3=C4H6+C2H6 3.980E+12

0.000 0.0 C2H3+C4H71-3=C2H4+C4H6 3.980E+12 0.000 0.0 C3H5-A+C4H71-3=C3H6+C4H6 6.310E+12 0.000 0.0 C4H71-3+C4H71-3=C8H141-5,3-4 4.110E+16 -1.260 1561.0 C4H71-3+C4H71-3=C8H141-5,3 4.110E+16 -1.260 1561.0 C4H71-3+C4H71-3=C8H142-6 4.110E+16 -1.260 1561.0 C8H141-5,3-4+OH=C8H131-5,3-4,TA+H2O 2.500E+06 2.000 -2629.0 C8H141-5,3+OH=C8H131-5,3,TA+H2O 1.300E+06 2.000 -2629.0 C8H141-5,3+OH=C8H131-5,3,SA+H2O 3.200E+06 2.000 -1434.0 C8H141-5,3+OH=C8H131-5,3,PA+H2O 3.000E+06 2.000 -239.0 C8H142-6+OH=C8H132-6,SA+H2O 6.300E+06 2.000 -1434.0 C8H142-6+OH=C8H132-6,PA+H2O 6.000E+06 2.000 -239.0 C8H141-5,3-4+HO2=C8H131-5,3-4,TA+H2O2 3.200E+04 2.600 10755.0 C8H141-5,3+HO2=C8H131-5,3,TA+H2O2 1.600E+04 2.600 10755.0 C8H141-5,3+HO2=C8H131-5,3,SA+H2O2 6.300E+03 2.600 12428.0 C8H141-5,3+HO2=C8H131-5,3,PA+H2O2 9.500E+03 2.600 13862.0 C8H142-6+HO2=C8H132-6,SA+H2O2 1.300E+04 2.600 12428.0 C8H142-6+HO2=C8H132-6,PA+H2O2 1.900E+04 2.600 13862.0 C8H141-5,3-4+H=C8H131-5,3-4,TA+H2 5.000E+04 2.500 -2868.0 C8H141-5,3+H=C8H131-5,3,TA+H2 2.500E+04 2.500 -2868.0 C8H141-5,3+H=C8H131-5,3,SA+H2 5.000E+04 2.500 -1673.0 C8H141-5,3+H=C8H131-5,3,PA+H2 1.900E+05 2.500 2390.0 C8H142-6+H=C8H132-6,SA+H2 1.000E+05 2.500 -1673.0 C8H142-6+H=C8H132-6,PA+H2 3.800E+05 2.500 2390.0 C8H141-5,3-4+O=C8H131-5,3-4,TA+OH 6.300E+10 0.700 1195.0 C8H141-5,3+O=C8H131-5,3,TA+OH 3.200E+10 0.700 1195.0 C8H141-5,3+O=C8H131-5,3,SA+OH 8.000E+10 0.700 3107.0 C8H141-5,3+O=C8H131-5,3,PA+OH 6.300E+10 0.700 5975.0 C8H142-6+O=C8H132-6,SA+OH 1.600E+11 0.700 3107.0 C8H142-6+O=C8H132-6,PA+OH 1.300E+11 0.700 5975.0 C8H141-5,3-4+CH3=C8H131-5,3-4,TA+CH4 1.600E+12 0.000 5258.0 C8H141-5,3+CH3=C8H131-5,3,TA+CH4 7.900E+11 0.000 5258.0 C8H141-5,3+CH3=C8H131-5,3,SA+CH4 1.600E+12 0.000 6931.0 C8H141-5,3+CH3=C8H131-5,3,PA+CH4 1.500E-01 3.500 5736.0 C8H142-6+CH3=C8H132-6,SA+CH4 3.200E+12 0.000 6931.0 C8H142-6+CH3=C8H132-6,PA+CH4 3.000E-01 3.500 5736.0 C8H141-5,3-4+O2=C8H131-5,3-4,TA+HO2 1.600E+13 0.000 35420.0 C8H141-5,3+O2=C8H131-5,3,TA+HO2 8.000E+12 0.000 35420.0 C8H141-5,3+O2=C8H131-5,3,SA+HO2 2.000E+13 0.000 37190.0 C8H141-5,3+O2=C8H131-5,3,PA+HO2 2.000E+13 0.000 39390.0 C8H142-6+O2=C8H132-6,SA+HO2 4.000E+13 0.000 37190.0 C8H142-6+O2=C8H132-6,PA+HO2 4.000E+13 0.000 39390.0 C6H101-3,3+C2H3=C8H131-5,3-4,TA 4.400E+04 2.480 6130.0 B13DE2M+C3H5-S=C8H131-5,3,TA 4.400E+04 2.480 6130.0 C6H10D24+C2H3=C8H131-5,3,SA 8.800E+03 2.480 6130.0 C4H6+C4H71-3=C8H131-5,3,PA 1.300E+03 2.480 8520.0 C5H81-3+C3H5-S=C8H132-6,SA 8.800E+03 2.480 6130.0 C4H6+C4H71-3=C8H132-6,PA 1.300E+03 2.480 8520.0 C6H101-3,3=C2H3+C4H72-2 2.500E+15 0.000 99500.0 C6H10D24=C3H5-S+C3H5-S 2.500E+15 0.000 118000.0 C8H131-5,3-4,TA+HO2=C8H131-5,3-4,TAO+OH 1.640E+04 2.740 1144.0 C8H131-5,3,TA+HO2=C8H131-5,3,TAO+OH 1.640E+04 2.740 1144.0 C8H131-5,3,SA+HO2=C8H131-5,3,SAO+OH 1.640E+04 2.740 1144.0 C8H131-5,3,PA+HO2=C8H131-5,3,PAO+OH 1.640E+04 2.740 1144.0 C8H132-6,SA+HO2=C8H132-6,SAO+OH 1.640E+04 2.740 1144.0 C8H132-6,PA+HO2=C8H132-6,PAO+OH 1.640E+04 2.740 1144.0 C4H71-3+C2H3COCH3=C8H131-5,3-4,TAO 2.500E+10 0.000

10090.0 C4H71-3+C2H3COCH3=C8H131-5,3,TAO 2.500E+10 0.000 10090.0 C4H71-3+SC3H5CHO=C8H131-5,3,SAO 3.330E+10 0.000 10597.0 C7H111-5,3,6P+CH2O=C8H131-5,3,PAO 1.000E+11 0.000 3496.0 C4H71-3+SC3H5CHO=C8H132-6,SAO 3.330E+10 0.000 10597.0 C7H111-5,1P+CH2O=C8H132-6,PAO 1.000E+11 0.000 3496.0 CC5H9-A+C2H2=C7H111-5,3,6P 1.320E+04 2.480 6130.0 C5H92-5+C2H2=C7H111-5,1P 1.320E+04 2.480 6130.0 C4H71-4+O2=C4H6+HO2 1.000E+11 0.000 0.0 C4H71-4+O2=C4H71-4O2 6.860E+16 -1.627 199.0 C4H71-4+HO2=C4H7O1-4+OH 7.000E+12 0.000 -1000.0 CH3O2+C4H71-4=CH3O+C4H7O1-4 7.000E+12 0.000 -1000.0 C4H71-4O2+H2=C4H71-4OOH+H 3.010E+13 0.000 26030.0 C4H71-4O2+HO2=C4H71-4OOH+O2 1.750E+10 0.000 -3275.0 C4H71-4O2+H2O2=C4H71-4OOH+HO2 2.400E+12 0.000 10000.0 C4H71-4O2+CH4=C4H71-4OOH+CH3 1.120E+13 0.000 24640.0 C4H71-4O2+CH3OH=C4H71-4OOH+CH2OH 6.300E+12 0.000 19360.0 C4H71-4O2+CH2O=C4H71-4OOH+HCO 5.600E+12 0.000 13600.0 C4H71-4O2+C2H6=C4H71-4OOH+C2H5 1.700E+13 0.000 20460.0 C4H71-4O2+CH3CHO=C4H71-4OOH+CH3CO 2.800E+12 0.000 13600.0 C4H71-4O2+C2H4=C4H71-4OOH+C2H3 1.130E+13 0.000 30430.0 C4H71-4O2+C3H6=C4H71-4OOH+C3H5-A 5.350E-02 4.207 13288.0 C4H71-4O2+C2H5CHO=C4H71-4OOH+C2H5CO 2.000E+11 0.000 9500.0 C4H71-4O2+C2H3CHO=C4H71-4OOH+C2H3CO 2.800E+12 0.000 13600.0 C4H71-4O2+C3H8=C4H71-4OOH+NC3H7 1.700E+13 0.000 20460.0 C4H71-4O2+C3H8=C4H71-4OOH+IC3H7 2.000E+12 0.000 17000.0 C4H71-4O2+CH3=C4H7O1-4+CH3O 7.000E+12 0.000 -1000.0 C4H71-4O2+C2H5=C4H7O1-4+C2H5O 7.000E+12 0.000 -1000.0 C4H71-4O2+IC3H7=C4H7O1-4+IC3H7O 7.000E+12 0.000 -1000.0 C4H71-4O2+NC3H7=C4H7O1-4+NC3H7O 7.000E+12 0.000 -1000.0 C4H71-4O2+C3H5-A=C4H7O1-4+C3H5O 7.000E+12 0.000 -1000.0 C4H71-4O2+PC4H9=C4H7O1-4+PC4H9O 7.000E+12 0.000 -1000.0 C4H71-4O2+SC4H9=C4H7O1-4+SC4H9O 7.000E+12 0.000 -1000.0 C4H71-4O2+C4H71-3=C4H7O1-4+C4H71-O 7.000E+12 0.000 -1000.0 C4H71-4OOH=C4H7O1-4+OH 1.500E+16 0.000 42500.0 C4H71-4O2+CH3O2=¿C4H7O1-4+CH3O+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+CH3CO3=¿C4H7O1-4+CH3CO2+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+C2H5O2=¿C4H7

4+C2H5O+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+NC3H7O2=¿C4H7O1-4+NC3H7O+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+IC3H7O2=¿C4H7O1-4+IC3H7O+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+C4H71-4O2=¿C4H7O1-4+C4H7O1-4+O2 1.400E+16 -1.610 1860.0 C4H71-4O2+SC4H9O2=¿C4H7O1-4+SC4H9O+O2 1.400E+16 -1.610 1860.0 C4H71-4O2=C4H61-3OOH4 4.010E+08 1.100 30100.0 C4H61-3OOH4=C2H3CHOCH2+OH 1.710E+09 1.060 10900.0 C4H61-3OOH4=C4H6O25+OH 1.720E+08 0.760 11100.0 C2H3CHOCH2+H=¿C2H3+CH2CO+H2 5.000E+12 0.000 0.0 C2H3CHOCH2+O=¿C2H3+CH2CO-

5.000E+12 0.000 0.0 C2H3CHOCH2+OH=¿C2H3+CH2CO+H2O 5.000E+12 0.000 0.0 C2H3CHOCH2+HO2=¿C2 1.000E+13 0.000 15000.0 C2H3CHOCH2+CH3=¿C2H3+CH2CO+CH4 2.000E+11 0.000 10000.0 C2H3CHOCH2+CH3O2=¿C2H3+CH2CO+CH3O2H 1.000E+13 0.000 19000.0 C4H6O25+H=CH2CHCHCHO+H2 5.000E+12 0.000 0.0 C4H6O25+O=CH2CHCHCHO+OH 5.000E+12 0.000 0.0 C4H6O25+OH=CH2CHCHCHO+H 5.000E+12 0.000 0.0 C4H6O25+HO2=CH2CHCHCHO+H2O2 1.000E+13 0.000 15000.0 C4H6O25+CH3=CH2CH 2.000E+11 0.000 10000.0 C4H6O25+CH3O2=CH2CHCHCHO+CH3O2H 1.000E+13 0.000 19000.0

C4H61-3OOH4+HO2=C4H6O1-3OOH4+OH 4.100E+03 2.740 1144.0 C4H61-3OOH4+HO2=C4H6O2-1OOH4+OH 4.100E+03 2.740 1144.0 C4H6O1-3OOH4=¿C2H3CHO+CH2O+OH 6.700E+39 -8.380 22782.0 C4H6O1-3OOH4=C2H3+HO2CH2CHO 2.670E+34 -6.630 22672.0 C4H71-1+O2=C4H71-1O2 4.070E+27 -4.670 5222.0 C4H71-1O2=C3H6CHO-3+O 1.220E+29 -4.710 42340.0 C4H71-1O2=C2H5CHCO+OH 1.550E+24 -3.870 49850.0 C4H71-2+O2=C4H71-2O2 4.070E+27 -4.670 5222.0 C4H71-2O2=C2H5COCH2+O 1.220E+29 -4.710 42340.0 C4H72-2+O2=C4H72-2O2 4.070E+27 -4.670 5222.0 C4H72-2O2=CH3CHCOCH3+O 1.220E+29 -4.710 42340.0 C4H8-1+H=C2H4+C2H5 1.000E+00 1.000 1.0 PLOG / 1.00E-03 2.550E+06 1.930 5564.0 / PLOG / 1.00E-02 5.560E+06 1.830 5802.0 / PLOG / 1.00E-01 1.210E+09 1.180 7472.0 / PLOG / 1.00E+00 9.470E+16 -1.030 13413.0 / PLOG / 1.00E+01 4.500E+28 -4.240 23618.0 / PLOG / 1.00E+02 7.020E+32 -5.220 31754.0 / DUP C4H8-1+H=C2H4+C2H5 1.000E+00 1.000 1.0 PLOG / 1.00E-03 3.450E+07 1.810 2263.0 / PLOG / 1.00E-02 8.060E+07 1.710 2522.0 / PLOG / 1.00E-01 1.180E+10 1.100 4077.0 / PLOG / 1.00E+00 6.020E+15 -0.490 8452.0 / PLOG / 1.00E+01 7.580E+21 -2.140 14245.0 / PLOG / 1.00E+02 2.290E+21 -1.870 17243.0 / DUP C4H8-1+H=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-03 7.830E+09 1.170 1442.0 / PLOG / 1.00E-02 3.390E+10 1.000 1895.0 / PLOG / 1.00E-01 3.700E+13 0.140 4127.0 / PLOG / 1.00E+00 4.570E+19 -1.540 9061.0 / PLOG / 1.00E+01 8.570E+23 -2.660 14140.0 / PLOG / 1.00E+02 1.320E+20 -1.460 15383.0 / DUP C4H8-1+H=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.800E+06 1.760 5900.0 / PLOG / 1.00E-02 3.460E+06 1.680 6100.0 / PLOG / 1.00E-01 4.020E+08 1.100 7574.0 / PLOG / 1.00E+00 1.210E+16 -0.990 13175.0 / PLOG / 1.00E+01 7.140E+27 -4.230 23319.0 / PLOG / 1.00E+02 1.000E+33 -5.490 31922.0 / DUP C4H8-1+H=PC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.350E+15 -2.810 1570.0 / PLOG / 1.00E-02 5.200E+16 -2.970 1992.0 / PLOG / 1.00E-01 1.910E+21 -3.970 4636.0 / PLOG / 1.00E+00 1.900E+31 -6.460 11968.0 / PLOG / 1.00E+01 2.100E+40 -8.600 21058.0 / PLOG / 1.00E+02 1.440E+37 -7.210 24896.0 / DUP C4H8-1+H=PC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 4.330E+20 -4.160 -263.0 / PLOG / 1.00E-02 1.780E+22 -4.330 186.0 / PLOG / 1.00E-01 1.980E+26 -5.180 2518.0 / PLOG / 1.00E+00 3.780E+32 -6.630 7265.0 / PLOG / 1.00E+01 8.790E+34 -6.910 10952.0 / PLOG / 1.00E+02 7.800E+28 -4.790 10355.0 / DUP C4H8-1+H=SC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 4.070E+22 -4.510 -771.0 / PLOG / 1.00E-02 3.900E+24 -4.780 -34.0 / PLOG / 1.00E-01 2.030E+29 -5.810 2970.0 / PLOG / 1.00E+00 3.530E+34 -6.950 7525.0 / PLOG / 1.00E+01 1.190E+34 -6.420 9810.0 / PLOG / 1.00E+02 1.370E+26 -3.790 8012.0 / DUP C4H8-1+H=SC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 3.520E+12 -2.150 1466.0 / PLOG / 1.00E-02 1.020E+14 -2.280 1799.0 / PLOG / 1.00E-01 1.160E+18 -3.130 4049.0 / PLOG / 1.00E+00 5.220E+27 -5.530 10963.0 / PLOG / 1.00E+01 4.330E+37 -7.920 20354.0 / PLOG / 1.00E+02 2.220E+36 -7.060 25203.0 / DUP C4H8-2+H=C2H4+C2H5 1.000E+00 1.000 1.0 PLOG / 1.00E-03 8.960E+06 1.860 6209.0 / PLOG / 1.00E-02 1.920E+07 1.770 6443.0 /

PLOG / 1.00E-01 3.970E+09 1.110 8097.0 / PLOG / 1.00E+00 3.010E+17 -1.090 14023.0 / PLOG / 1.00E+01 1.880E+29 -4.330 24297.0 / PLOG / 1.00E+02 5.150E+33 -5.390 32601.0 / C4H8-2+H=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-03 6.390E+09 1.290 1834.0 / PLOG / 1.00E-02 2.600E+10 1.120 2267.0 / PLOG / 1.00E-01 2.480E+13 0.290 4456.0 / PLOG / 1.00E+00 2.910E+19 -1.390 9365.0 / PLOG / 1.00E+01 6.130E+23 -2.530 14463.0 / PLOG / 1.00E+02 1.230E+20 -1.350 15762.0 / C4H8-2+H=PC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 3.900E+14 -2.550 1729.0 / PLOG / 1.00E-02 1.410E+16 -2.710 2133.0 / PLOG / 1.00E-01 4.310E+20 -3.690 4719.0 / PLOG / 1.00E+00 4.030E+30 -6.170 12020.0 / PLOG / 1.00E+01 5.190E+39 -8.330 21137.0 / PLOG / 1.00E+02 5.170E+36 -6.980 25063.0 / C4H8-2+H=SC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 8.340E+21 -4.210 -602.0 / PLOG / 1.00E-02 6.790E+23 -4.460 82.0 / PLOG / 1.00E-01 2.850E+28 -5.470 3003.0 / PLOG / 1.00E+00 5.450E+33 -6.610 7559.0 / PLOG / 1.00E+01 2.330E+33 -6.110 9893.0 / PLOG / 1.00E+02 3.270E+25 -3.510 8145.0 / C4H8-1+H=C4H8-2+H 1.000E+00 1.000 1.0 PLOG / 1.00E-03 2.980E+07 1.860 3575.0 / PLOG / 1.00E-02 6.110E+07 1.770 3794.0 / PLOG / 1.00E-01 4.780E+09 1.240 5152.0 / PLOG / 1.00E+00 1.020E+15 -0.250 9233.0 / PLOG / 1.00E+01 6.510E+20 -1.820 14806.0 / PLOG / 1.00E+02 4.440E+19 -1.370 17409.0 / DUP C4H8-1+H=C4H8-2+H 1.000E+00 1.000 1.0 PLOG / 1.00E-03 1.550E+04 2.320 7049.0 / PLOG / 1.00E-02 2.360E+04 2.270 7177.0 / PLOG / 1.00E-01 6.600E+05 1.860 8201.0 / PLOG / 1.00E+00 1.150E+12 0.110 12789.0 / PLOG / 1.00E+01 8.800E+23 -3.170 22546.0 / PLOG / 1.00E+02 3.720E+31 -5.160 32234.0 / DUP SC4H9=PC4H9 1.000E+00 1.000 1.0 PLOG / 1.00E-03 9.600E+37 -11.040 38840.0 / PLOG / 1.00E-02 6.050E+40 -11.260 39461.0 / PLOG / 1.00E-01 1.640E+47 -12.490 43112.0 / PLOG / 1.00E+00 6.530E+55 -14.270 50351.0 / PLOG / 1.00E+01 2.130E+56 -13.710 54866.0 / PLOG / 1.00E+02 6.020E+45 -10.070 53399.0 / PC4H9=C2H4+C2H5 1.000E+00 1.000 1.0 PLOG / 1.00E-03 3.440E+34 -8.100 28397.0 / PLOG / 1.00E-02 1.110E+39 -9.050 31891.0 / PLOG / 1.00E-01 7.740E+42 -9.780 35771.0 / PLOG / 1.00E+00 7.470E+43 -9.670 38722.0 / PLOG / 1.00E+01 2.060E+39 -7.970 38955.0 / PLOG / 1.00E+02 1.480E+29 -4.710 35950.0 / PC4H9=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-03 3.710E+25 -5.810 34965.0 / PLOG / 1.00E-02 1.850E+27 -6.010 35481.0 / PLOG / 1.00E-01 2.460E+32 -7.160 38637.0 / PLOG / 1.00E+00 2.050E+42 -9.610 46415.0 / PLOG / 1.00E+01 4.980E+48 -10.970 54456.0 / PLOG / 1.00E+02 2.230E+42 -8.680 56601.0 / SC4H9=C2H4+C2H5 1.000E+00 1.000 1.0 PLOG / 1.00E-03 8.300E+25 -5.750 39343.0 / PLOG / 1.00E-02 4.120E+27 -5.940 39859.0 / PLOG / 1.00E-01 5.570E+32 -7.100 43029.0 / PLOG / 1.00E+00 4.540E+42 -9.540 50839.0 / PLOG / 1.00E+01 1.060E+49 -10.900 58899.0 / PLOG / 1.00E+02 9.940E+42 -8.700 61203.0 / SC4H9=C3H6+CH3 1.000E+00 1.000 1.0 PLOG / 1.00E-03 2.890E+40 -9.760 33601.0 / PLOG / 1.00E-02 1.800E+44 -10.500 37007.0 / PLOG / 1.00E-01 2.510E+46 -10.730 40237.0 / PLOG / 1.00E+00 4.740E+44 -9.850 41841.0 / PLOG / 1.00E+01 3.790E+37 -7.440 40604.0 / PLOG / 1.00E+02 4.790E+26 -4.010 36898.0 /

C4H71-1OH+H=PC4H8OH-1 4.270E+12 0.493 4445.0 NC3H7CHO+H=PC4H8OH-1 9.800E+10 1.192 8786.0 C2H3OH+C2H5=PC4H8OH-1 3.000E+06 1.834 7338.0 C4H8-1+OH=PC4H8OH-2 2.100E+06 1.806 -3292.0 C4H71-1OH+H=PC4H8OH-2 1.600E+10 1.114 4389.0 C4H72-1OH+H=PC4H8OH-2 2.700E+11 -0.134 1585.0 C3H6+CH2OH=PC4H8OH-3 7.000E+03 2.427 7064.0 C4H71-4OH+H=PC4H8OH-3 1.500E+11 0.883 2751.0 SC4H8OH-1=PC4H8OH-3 2.900E+08 1.377 37866.0 C3H6+CH2OH=PC4H8OH-4 7.000E+03 2.427 7064.0 C4H71-4OH+H=PC4H8OH-4 1.500E+11 0.883 2751.0 SC4H8OH-1=PC4H8OH-4 2.900E+08 1.377 37866.0 NC3H7CHO+H=PC4H9O 4.700E+09 1.435 4358.0 NC3H7+CH2O=PC4 5.000E+03 2.425 3239.0 C4H71-2OH+H=SC4H8OH-2 1.400E+08 1.516 219.0 C2H5COCH3+H=SC4H8OH-2 7.000E+07 1.801 13223.0 C4H8-1+OH=SC4H8OH-1 7.000E+05 1.802 -3290.0 C2H3OH+C2H5=SC4H8OH-1 6.400E+06 1.671 10270.0 C4H8-2+OH=SC4H8OH-3 1.400E+06 1.802 -3290.0 SC3H5OH+CH3=SC4H8OH-3 6.400E+06 1.671 10270.0 C2H5COCH3+H=SC4H9O 2.700E+07 1.756 6206.0 C2H5CHO+CH3=SC4H9O 1.200E+04 2.284 7978.0 C4H71-4OH+OH=C4H64,2-1OH+H2O 2.020E+06 2.200 -437.0 C4H71-4OH+HO2=C4H64,2-1OH+H2O2 3.910E-01 3.970 11702.0 PC4H8OH-2+O2=PC4H8OH-2O2 3.600E+12 0.000 0.0 PC4H8OH-2O2=SQC4H8OP 2.910E+12 -0.226 22300.0 PC4H8OH-2O2=C4H72-1OH+HO2 3.640E+14 -0.711 32710.0 PC4H8OH-2O2=C4H71-1OH+HO2 2.440E+13 -0.253 32590.0 SQC4H8OP=¿C2H5CHO 5.360E+12 -0.080 10790.0 PC4H8OH-2O2=NC4KET21OH+OH 1.490E+09 0.109 41390.0 C4H72-1OH+OH=C4H64,2-1OH+H2O 2.020E+06 2.200 -437.0 C4H72-1OH+OH=C4H63,1-1OH+H2O 2.690E+06 2.200 -437.0 C4H72-1OH+HO2=C4H64,2-1OH+H2O2 1.720E-01 4.000 12103.0 C4H72-1OH+HO2=C4H63,1-1OH+H2O2 2.300E-01 4.000 12103.0 C4H71-1OH+OH=C4H63,1-1OH+H2O 2.020E+06 2.200 -437.0 C4H71-1OH+HO2=C4H63,1-1OH+H2O2 3.910E-01 3.970 11702.0 C4H64,2-1OH=C4H6+OH 7.040E+16 -1.012 36070.0 C4H63,1-1OH=C4H5OH-13+H 7.720E+12 0.488 43940.0 C4H5OH-13=C4H5-N+OH 5.610E+21 -1.612 106000.0 C4H5OH-13=C2H3+CH2CHO 2.820E+24 -2.381 90130.0 NC4KET21OH+OH=C2H4COCH2OH+H2O 8.450E+11 0.000 -228.0 NC4KET21OH+HO2=C2H4 2.000E+11 0.000 8698.0 NC4KET21OH+O=C2H4COCH2OH+OH 3.070E+13 0.000 3400.0 NC4KET21OH+H=C2 4.460E+06 2.000 3200.0 NC4KET21OH+O2=C2H4COCH2OH+HO2 1.550E+13 0.000 41970.0 NC4KET21OH+CH3=C2H4COCH2OH+CH4 1.740E+00 3.460 3680.0 NC4KET21OH+CH3O=C2H4COCH2OH+ 1.450E+11 0.000 2771.0 NC4KET21OH+CH3O2=C2H4COCH2OH+CH3O2H 2.000E+12 0.000 15250.0 NC4KET21OH+C2H3=C2H4COCH2OH+C2H4 3.000E+11 0.000 3400.0 NC4KET21OH+C2H5=C2H4CO 3.000E+10 0.000 8600.0 C2H4COCH2OH=CH3CHCO+CH2OH 9.440E+29 -4.930 38330.0 PC4H8OH-2O2=SQC4H7OHP-4 1.440E+07 1.400 20800.0 SQC4H7OHP-4=CY(CCCO)COH+OH 2.440E+09 0.780 18000.0 SQC4H7OHP-4=¿OH+HOCH2CHO+C2H4 3.080E+08 1.500 23500.0 CY(CCCO)COH+H=¿C2H4+ 5.000E+12 0.000 0.0 CY(CCCO)COH+O=¿C2H4+HOCH2CO+OH 5.000E+12 0.000 0.0 CY(CCCO)COH+OH=¿C 5.000E+12 0.000 0.0 CY(CCCO)COH+HO2=¿C2H4+HOCH2CO+H2O2 1.000E+13 0.000 15000.0 CY(CCCO)COH+CH3=¿C2H4+HOCH2CO+CH4 2.000E+11 0.000 10000.0 CY(CCCO)COH+CH3O2=¿C2H4+HO 1.000E+13 0.000 19000.0 CY(CCCO)COH+H=¿CH2O+CH2CCH2OH+H2 5.000E+12 0.000 0.0 CY(CCCO)COH+O=¿CH2O+CH2CCH2OH+OH 5.000E+12 0.000 0.0 CY(CCCO)COH+OH=¿CH2O+CH2CCH2

5.000E+12 0.000 0.0 CY(CCCO)COH+HO2=¿CH2O+CH2CCH2OH+H2O2 1.000E+13 0.000 15000.0
CY(CCCO)COH+CH3=¿CH2O+CH2CCH2OH+CH4 2.000E+11 0.000 10000.0 CY(CCCO)COH+CH3O2=¿CH2O
1.000E+13 0.000 19000.0 HOCH2CO=CH2OH+CO 1.070E+12 0.630 16900.0 SQC4H7OHP-4+O2=SQC4H7OHP-
4O2 3.430E+16 -1.627 199.0 SQC4H7OHP-4O2=C4H6OHOOH1-4-3+HO2 1.440E+07 1.380 28900.0
SQC4H7OHP-4O2=NC4KET24OH-1+OH 5.790E+01 2.900 17000.0 C4H6OHOOH1-4-3=¿C2H3CHO+CH2OH+C
1.050E+16 0.000 41600.0 C4H6OHOOH1-4-3=¿HOCH2CHO+C2H3+OH 1.050E+16 0.000 41600.0
NC4KET24OH-1=¿CH2O+HOCH2COCH2+OH 1.500E+16 0.000 43000.0 HOCH2CHO+O2=HOCH2CO+HO2
3.010E+13 0.000 39150.0 HOCH2CHO+O=HOCH2CO+OH 5.940E+12 0.000 1868.0 HOCH2CHO+H=HOCH2CO
1.310E+05 2.580 1220.0 HOCH2CHO+OH=HOCH2CO+H2O 3.370E+12 0.000 -619.0 HOCH2CHO+HO2=HOCH
3.010E+12 0.000 11920.0 HOCH2CHO+CH3=HOCH2CO+CH4 7.080E-04 4.580 1966.0 HOCH2CHO+CH3O2=HO
3.010E+12 0.000 11920.0 HOCH2CHO+CH3CO3=HOCH2CO+CH3CO3H 3.010E+12 0.000 11920.0
SC4H8OH-1+O2=SC4H8OH-1O2 3.600E+12 0.000 0.0 SC4H8OH-1O2=PQC4H8OS 9.300E+10 -
0.036 22890.0 SC4H8OH-1O2=NC4KET12OH+OH 1.490E+09 0.109 41390.0 PQC4H8OS=¿C2H5CHO+CH2O+C
6.700E+39 -8.380 22782.0 PQC4H8OS=¿C2H5+HO2CH2CHO 2.670E+34 -6.630 22672.0 SC4H8OH-
1O2=C4H71-2OH+HO2 2.440E+13 -0.253 32590.0 SC4H8OH-1O2=PQC4H7OHS-3 1.360E+07
1.300 18200.0 PQC4H7OHS-3=CCY(COCC)OH+OH 2.590E+09 0.690 16000.0 PQC4H7OHS-3=¿OH+CH2O+SC
1.230E+09 1.300 24900.0 C4H71-2OH+OH=C4H63,1-2OH+H2O 2.020E+06 2.200 -437.0 C4H71-
2OH+HO2=C4H63,1-2OH+H2O2 3.910E-01 3.970 11702.0 C4H63,1-2OH=C4H612+OH 1.000E+15
0.000 62900.0 NC4KET12OH+H=C2H5CHOHCO+H2 1.000E+05 2.580 1220.0 NC4KET12OH+OH=C2H5CHOH
1.700E+12 0.000 -619.0 NC4KET12OH+O=C2H5CHOHCO+OH 5.940E+12 0.000 1868.0 NC4KET12OH+HO2=C
9.500E+03 2.700 11520.0 NC4KET12OH+CH3=C2H5CHOHCO+CH4 1.420E-03 4.580 1966.0 NC4KET12OH+C2
7.360E+04 2.000 5917.0 NC4KET12OH+CH3O=C2H5CHOHCO+CH3OH 1.000E+12 0.000 3300.0
NC4KET12OH+CH3O2=C2H5CHOHCO+CH3O2H 3.010E+12 0.000 11920.0 NC4KET12OH+O2=C2H5CHOHC
9.030E+13 0.000 43320.0 NC4KET12OH+C2H3=C2H5CHOHCO+C2H4 3.260E+05 2.000 3966.0
NC4KET12OH+C2H5O=C2H5CHOHCO+C2H5OH 6.030E+11 0.000 3300.0 C2H5CHOHCO=C3H6OH1-
1+CO 5.780E+14 0.000 16844.0 C3H6OH1-1=C2H5CHO+H 8.980E+11 0.271 32990.0 C2H3OH+CH3=C3H6OH1
1 2.040E+40 -8.250 24214.0 DUP C2H3OH+CH3=C3H6OH1-1 1.660E+21 -3.170 10241.0 DUP
CCY(COCC)OH+H=¿OH+C2H3COCH3+H2 5.000E+12 0.000 0.0 CCY(COCC)OH+O=¿OH+C2H3COCH3+OH
5.000E+12 0.000 0.0 CCY(COCC)OH+OH=¿OH+C2H3COCH3+H2O 5.000E+12 0.000 0.0 CCY(COCC)OH+HO2
1.000E+13 0.000 15000.0 CCY(COCC)OH+CH3=¿OH+C2H3COCH3+CH4 2.000E+11 0.000 10000.0
CCY(COCC)OH+CH3O2=¿OH+C2H3COCH3+CH3O2H 1.000E+13 0.000 19000.0 CCY(COCC)OH+H=¿OH+SC
5.000E+12 0.000 0.0 CCY(COCC)OH+O=¿OH+SC3H5CHO+OH 5.000E+12 0.000 0.0 CCY(COCC)OH+OH=¿O
5.000E+12 0.000 0.0 CCY(COCC)OH+HO2=¿OH+SC3H5CHO+H2O2 1.000E+13 0.000 15000.0
CCY(COCC)OH+CH3=¿OH+SC3H5CHO+CH4 2.000E+11 0.000 10000.0 CCY(COCC)OH+CH3O2=¿OH+SC3H
1.000E+13 0.000 19000.0 CCY(COCC)OH+H=¿C2H3OH+CH3CO+H2 5.000E+12 0.000 0.0 CCY(COCC)OH+O=
5.000E+12 0.000 0.0 CCY(COCC)OH+OH=¿C2H3OH+CH3CO+H2O 5.000E+12 0.000 0.0 CCY(COCC)OH+HO2

1.000E+13 0.000 15000.0 CCY(COCC)OH+CH3=¿C2H3OH+CH3CO+CH4 2.000E+11 0.000 10000.0
CCY(COCC)OH+CH3O2=¿C2H3OH+CH3CO+CH3O2H 1.000E+13 0.000 19000.0 CCY(COCC)OH+H=¿HCO+S
5.000E+12 0.000 0.0 CCY(COCC)OH+O=¿HCO+SC3H5OH+OH 5.000E+12 0.000 0.0 CCY(COCC)OH+OH=¿H
5.000E+12 0.000 0.0 CCY(COCC)OH+HO2=¿HCO+SC3H5OH+H2O2 1.000E+13 0.000 15000.0
CCY(COCC)OH+CH3=¿HCO+SC3H5OH+CH4 2.000E+11 0.000 10000.0 CCY(COCC)OH+CH3O2=¿HCO+SC3
1.000E+13 0.000 19000.0 PQC4H7OHS-3+O2=PQC4H7OHS-3O2 1.740E+14 -0.816 -536.0 PQC4H7OHS-
3O2=NC4KET13OH-2+OH 1.090E+04 2.400 19900.0 NC4KET13OH-2=¿CH3CHO+HOCHCHO+OH
1.050E+16 0.000 43000.0 PQC4H7OHS-3O2=C4H7O2-1,3OOH 2.910E+12 -0.226 22300.0 PQC4H7OHS-
3O2=C4H6OHOOH1-3-4+HO2 3.640E+14 -0.711 32710.0 PQC4H7OHS-3O2=C4H6OHOOH2-2-
1+HO2 2.440E+13 -0.253 32590.0 C4H7O2-1,3OOH=¿C3KET12+CH2O+OH 5.360E+12 -0.080
10790.0 C4H7O2-1,3OOH=¿HO2CH2CHO+CH3CHO+OH 6.700E+39 -8.380 22782.0 PQC4H7OHS-
3O2=NC4KET24OH-3+OH 1.490E+09 0.109 41390.0 HOCHCHO+O=CHOCHO+OH 1.460E-03
4.730 1727.0 HOCHCHO+OH=CHOCHO+H2O 5.810E-03 4.280 -3560.0 HOCHCHO+H=CHOCHO+H2
9.450E+02 3.140 8701.0 HOCHCHO+HO2=CHOCHO+H2O2 6.470E-07 5.300 10533.0 HOCHCHO+CH3=CHOCH
2.040E+00 3.570 7721.0 HOCHCHO+CH3O2=CHOCHO+CH3O2H 3.240E-07 5.300 10533.0 C4H6OHOOH1-
3-4=¿CH2O+PC3H4OH-3+OH 1.500E+16 0.000 42000.0 C4H6OHOOH2-2-1=¿CH2O+PC3H4OH-
1+OH 1.500E+16 0.000 42000.0 NC4KET24OH-3=¿CH2O+CH3COCHOH+OH 1.500E+16 0.000
43000.0 PC3H4OH-3=C3H5O 5.480E+45 -11.630 44328.0 PC3H4OH-3=CH2CCH2OH 2.650E+36
-8.860 51019.0 PC3H4OH-3+O2=C2H3CHO+HO2 5.260E+17 -1.638 869.0 PC3H4OH-1=CH3CHCO+H
5.690E+52 -13.380 45049.0 PC3H4OH-1=PC3H4OH-2 2.650E+36 -8.860 51019.0 PC3H4OH-1+O2=CH3CHCO+H
5.260E+17 -1.638 869.0 CH3COCHOH=C3Y12+H 5.690E+52 -13.380 45049.0 CH3COCHOH=CH3COCH2O
5.480E+45 -11.630 44328.0 CH3COCHOH+O2=C3Y12+HO2 5.260E+17 -1.638 869.0 SC4H8OH-
3+O2=SC4H8OH-3O2 3.600E+12 0.000 0.0 SC4H8OH-3O2=SQC4H8OS 2.910E+12 -0.226 22300.0
SC4H8OH-3O2=C4H71-3OH+HO2 3.640E+14 -0.711 32710.0 SC4H8OH-3O2=C4H72-2OH+HO2
2.440E+13 -0.253 32590.0 SQC4H8OS=¿CH3CHO+CH3CHO+OH 2.680E+13 -0.080 10790.0 SC4H8OH-
3O2=NC4KET23OH+OH 1.490E+09 0.109 41390.0 SC4H8OH-3O2=SQC4H7OHS-4 1.440E+07
1.400 20800.0 SQC4H7OHS-4=CCY(COCC)OH+OH 2.440E+09 0.780 18000.0 SQC4H7OHS-4=¿OH+CH3CHO+
3.080E+08 1.500 23500.0 C4H71-3OH+OH=C4H63,1-3OH+H2O 2.020E+06 2.200 -437.0 C4H71-
3OH+HO2=C4H63,1-3OH+H2O2 3.910E-01 3.970 11702.0 C4H72-2OH+OH=C4H63,1-3OH+H2O
2.020E+06 2.200 -437.0 C4H72-2OH+HO2=C4H63,1-3OH+H2O2 3.910E-01 3.970 11702.0 C4H63,1-
3OH=C4H6+OH 7.040E+16 -1.012 36070.0 NC4KET23OH+OH=CH3COCOHCH3+H2O 8.450E+11
0.000 -228.0 NC4KET23OH+HO2=CH3COCOHCH3+H2O2 2.000E+11 0.000 8698.0 NC4KET23OH+O=CH3COC
3.070E+13 0.000 3400.0 NC4KET23OH+H=CH3COCOHCH3+H2 4.460E+06 2.000 3200.0 NC4KET23OH+O2=C
1.550E+13 0.000 41970.0 NC4KET23OH+CH3=CH3COCOHCH3+CH4 1.740E+00 3.460 3680.0
NC4KET23OH+CH3O=CH3COCOHCH3+CH3OH 1.450E+11 0.000 2771.0 NC4KET23OH+CH3O2=CH3COCOH
2.000E+12 0.000 15250.0 NC4KET23OH+C2H3=CH3COCOHCH3+C2H4 3.000E+11 0.000 3400.0

NC4KET23OH+C2H5=CH3COCOHCH3+C2H6 3.000E+10 0.000 8600.0 CH3COHCO+CH3=CH3COCOHCH3
1.230E+11 0.000 7800.0 CH3COHCO+OH=SC2H4OH+CO2 1.730E+12 0.000 -1010.0 CH3COHCO+H=SC2H4OH
4.400E+12 0.000 1459.0 SQC4H7OHS-4+O2=SQC4H7OHS-4O2 3.430E+16 -1.627 199.0 SQC4H7OHS-
4O2=NC4KET24OH-3+OH 5.790E+01 2.900 17000.0 SQC4H7OHS-4O2=C4H7O2-1,3OOH 9.300E+10
-0.036 22890.0 SQC4H7OHS-4O2=C4H6OHOOH1-2-3+HO2 2.440E+13 -0.253 32590.0 SQC4H7OHS-
4O2=NC4KET13OH-2+OH 1.490E+09 0.109 41390.0 C4H6OHOOH1-2-3=¿CH2COHCHO+CH3+OH
1.050E+16 0.000 41600.0 C4H6OHOOH1-2-3=¿CH3CHO+SC2H2OH+OH 1.050E+16 0.000 41600.0
SC2H2OH+HCO=CH2COHCHO 1.810E+13 0.000 0.0 CH2COHCHO+H=CH2COHCO+H2 1.340E+13
0.000 3300.0 CH2COHCHO+O=CH2COHCO+OH 5.940E+12 0.000 1868.0 CH2COHCHO+OH=CH2COHCO+H2
9.240E+06 1.500 -962.0 CH2COHCHO+O2=CH2COHCO+HO2 1.000E+13 0.000 40700.0 CH2COHCHO+HO2=C
3.010E+12 0.000 11920.0 CH2COHCHO+CH3=CH2COHCO+CH4 2.610E+06 1.780 5911.0 CH2COHCHO+C2H3
1.740E+12 0.000 8440.0 CH2COHCHO+CH3O=CH2COHCO+CH3OH 1.000E+12 0.000 3300.0
CH2COHCHO+CH3O2=CH2COHCO+CH3O2H 3.010E+12 0.000 11920.0 SC2H2OH+CO=CH2COHCO
1.510E+11 0.000 4810.0 SC2H2OH=CH2CO+H 5.690E+52 -13.380 45049.0 SC2H2OH=HCCOH+H
5.400E+46 -11.630 44323.0 SC2H2OH=C2H2OH 2.650E+36 -8.860 51019.0 SC2H2OH+O2=CH2CO+HO2
5.260E+17 -1.638 869.0 SC2H2OH+O2=HCCOH+HO2 5.510E+03 2.495 -414.0 C4H8-1+O=NC3H7+HCO
7.450E+06 1.880 183.0 C4H8-1+O=¿CH2CO+C2H5+H 3.050E+06 1.880 183.0 C4H8-1+O=¿C2H5CHCO+H+H
3.050E+06 1.880 183.0 C4H8-2+O=CH3+C2H5CO 7.450E+06 1.880 183.0 C4H8-2+O=¿CH2CO+C2H5+H
3.050E+06 1.880 183.0 C4H8-2+O=¿C2H5CHCO+H+H 3.050E+06 1.880 183.0 SC4H9O2=C4H8-
2+HO2 7.250E+09 0.800 29900.0 DUP SC4H9O2=C4H8-2+HO2 1.700E+10 0.670 30700.0 DUP
C4H8OOH1-2=C4H8-1+HO2 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.090E+13 -1.380 9113.0
/ PLOG / 1.00E-01 2.930E+18 -2.600 13142.0 / PLOG / 1.00E+00 7.800E+24 -4.050 18999.0
/ PLOG / 2.00E+00 1.760E+26 -4.320 20657.0 / PLOG / 5.00E+00 7.860E+26 -4.350 22246.0
/ PLOG / 1.00E+01 1.730E+26 -4.060 22736.0 / PLOG / 3.00E+01 1.390E+23 -3.040 22032.0
/ PLOG / 5.00E+01 1.450E+21 -2.430 21227.0 / C4H8-1+HO2=C4H8OOH2-1 1.460E-01 3.450
5798.0 PLOG / 1.33E-02 9.740E+05 0.410 7570.0 / PLOG / 1.00E+00 8.430E+14 -1.760 12124.0
/ PLOG / 1.00E+01 1.820E+20 -3.030 16135.0 / PLOG / 1.00E+02 8.790E+17 -2.040 17111.0 /
C4H8-1+HO2=C4H8O1-2+OH 1.000E+11 0.000 0.0 PLOG / 1.33E-02 2.960E+03 2.450 12199.0
/ PLOG / 1.00E+00 1.690E+10 0.510 16606.0 / PLOG / 1.00E+01 2.190E+17 -1.480 22209.0 /
PLOG / 1.00E+02 2.730E+21 -2.510 27857.0 / C4H8OOH2-1=C4H8O1-2+OH 3.920E+06 1.650
12124.0 PLOG / 1.33E-02 2.750E+22 -4.390 12349.0 / PLOG / 1.00E+00 2.440E+29 -5.900
17573.0 / PLOG / 1.00E+01 1.520E+30 -5.840 19702.0 / PLOG / 1.00E+02 1.930E+20 -2.660
16454.0 / C4H8-2+HO2=C4H8OOH2-3 9.550E+03 2.580 10347.0 PLOG / 1.33E-02 2.530E+12
-1.270 10098.0 / PLOG / 1.00E+00 1.340E+11 -0.480 8480.0 / PLOG / 1.00E+01 1.930E+17
-2.040 12122.0 / PLOG / 1.00E+02 4.450E+19 -2.450 14812.0 / C4H8-2+HO2=C4H8O2-3+OH
1.000E+11 0.000 0.0 PLOG / 1.33E-02 7.650E+05 1.926 10745.0 / PLOG / 1.00E+00 1.790E+08

1.251 12370.0 / PLOG / 1.00E+01 1.750E+15 -0.740 17220.0 / PLOG / 1.00E+02 8.370E+20 -
2.283 22838.0 / C4H8OOH2-3=C4H8O2-3+OH 1.050E+10 0.680 11964.0 PLOG / 1.33E-02 3.020E+19
-3.510 9746.0 / PLOG / 1.00E+00 6.370E+24 -4.550 13480.0 / PLOG / 1.00E+01 1.390E+28
-5.250 16470.0 / PLOG / 1.00E+02 1.540E+27 -4.690 17832.0 / C4H8-1+CH3O2=C4H8O1-
2+CH3O 1.000E+12 0.000 14340.0 C4H8-2+CH3O2=C4H8O2-3+CH3O 5.620E+11 0.000 12310.0
C4H6=C4H5-I+H 5.700E+36 -6.270 112353.0 C4H6=C4H5-N+H 5.300E+44 -8.620 123608.0 C4H6=C4H4+H2
2.500E+15 0.000 94700.0 H2CC+C2H4=C4H6 1.000E+12 0.000 0.0 C4H6+H=C4H5-N+H2 1.330E+06
2.530 12240.0 C4H5-N+HO2=C4H6+O2 6.000E+11 0.000 0.0 C4H6+O=C4H5-N+OH 7.500E+06
1.900 3740.0 C4H6+OH=C4H5-N+H2O 6.200E+06 2.000 3430.0 C4H5-N+H2O2=C4H6+HO2
1.210E+10 0.000 -596.0 C4H6+CH3=C4H5-N+CH4 2.000E+14 0.000 22800.0 C4H6+C2H3=C4H5-
N+C2H4 5.000E+13 0.000 22800.0 C4H6+C3H3=C4H5-N+C3H4-A 1.000E+13 0.000 22500.0
C4H6+C3H5-A=C4H5-N+C3H6 1.000E+13 0.000 22500.0 C4H6+H=C4H5-I+H2 6.650E+05 2.530
9240.0 C4H5-I+HO2=C4H6+O2 6.000E+11 0.000 0.0 C4H6+O=C4H5-I+OH 7.500E+06 1.900
3740.0 C4H6+OH=C4H5-I+H2O 3.100E+06 2.000 430.0 C4H5-I+H2O2=C4H6+HO2 1.210E+10
0.000 -596.0 C4H6+CH3=C4H5-I+CH4 1.000E+14 0.000 19800.0 C4H6+C2H3=C4H5-I+C2H4
2.500E+13 0.000 19800.0 C4H6+C3H3=C4H5-I+C3H4-A 5.000E+12 0.000 19500.0 C4H6+C3H5-
A=C4H5-I+C3H6 5.000E+12 0.000 19500.0 C4H6+H=C2H4+C2H3 1.460E+30 -4.340 21647.0
PLOG / 1.00E+00 1.460E+30 -4.340 21647.0 / PLOG / 1.00E+01 5.450E+30 -4.510 21877.0
/ C4H6+H=C3H4-P+CH3 2.000E+12 0.000 7000.0 C4H6+H=C3H4-A+CH3 2.000E+12 0.000
7000.0 C4H6+O=C2H2+C2H4O1-2 1.000E+08 1.450 -860.0 C4H6+O=SC3H5CO+H 5.000E+07
1.450 -860.0 C4H6+O=CH2CHCHCHO+H 4.500E+08 1.450 -860.0 C4H6+OH=C2H3CHO+CH3
1.370E+12 0.000 -1040.0 C4H6+OH=C3H5-A+CH2O 1.370E+12 0.000 -1040.0 C4H6+HO2=C4H6O25+OH
1.200E+12 0.000 14000.0 C4H6+HO2=C2H3CHOCH2+OH 4.800E+12 0.000 14000.0 C4H6O25=C4H4O+H2
5.300E+12 0.000 48500.0 C2H3CHOCH2=C4H6O23 2.000E+14 0.000 50600.0 C4H6O23=SC3H5CHO
1.950E+13 0.000 49400.0 C4H6O23=C2H4+CH2CO 5.750E+15 0.000 69300.0 C4H6O23=C2H2+C2H4O1-
2 1.000E+16 0.000 75800.0 C4H4O=CO+C3H4-P 1.780E+15 0.000 77500.0 C4H4O=C2H2+CH2CO
5.010E+14 0.000 77500.0 C2H3+C2H2=C4H4+H 2.000E+18 -1.680 10600.0 PLOG / 1.32E-02
7.200E+13 -0.480 6100.0 / PLOG / 2.63E-02 5.000E+14 -0.710 6700.0 / PLOG / 1.20E-01
4.600E+16 -1.250 8400.0 / PLOG / 1.00E+00 2.000E+18 -1.680 10600.0 / PLOG / 1.00E+01
4.900E+16 -1.130 11800.0 / C2H3+C2H2=C4H5-N 9.300E+38 -8.760 12000.0 PLOG / 1.32E-
02 1.100E+31 -7.140 5600.0 / PLOG / 2.63E-02 1.100E+32 -7.330 6200.0 / PLOG / 1.20E-01
2.400E+31 -6.950 5600.0 / PLOG / 1.00E+00 9.300E+38 -8.760 12000.0 / PLOG / 1.00E+01
8.100E+37 -8.090 13400.0 / C2H3+C2H2=C4H5-I 1.600E+46 -10.980 18600.0 PLOG / 1.32E-
02 5.000E+34 -8.420 7900.0 / PLOG / 2.63E-02 2.100E+36 -8.780 9100.0 / PLOG / 1.20E-01
1.000E+37 -8.770 9800.0 / PLOG / 1.00E+00 1.600E+46 -10.980 18600.0 / PLOG / 1.00E+01
5.100E+53 -12.640 28800.0 / C2H3+C2H3=C4H6 1.500E+42 -8.840 12500.0 PLOG / 2.63E-02

7.000E+57 -13.820 17600.0 / PLOG / 1.20E-01 1.500E+52 -11.970 16100.0 / PLOG / 1.00E+00
1.500E+42 -8.840 12500.0 / C2H3+C2H3=C4H5-I+H 1.200E+22 -2.440 13700.0 PLOG / 2.63E-
02 1.500E+30 -4.950 13000.0 / PLOG / 1.20E-01 7.200E+28 -4.490 14300.0 / PLOG / 1.00E+00
1.200E+22 -2.440 13700.0 / C2H3+C2H3=C4H5-N+H 2.400E+20 -2.040 15400.0 PLOG / 2.63E-
02 1.100E+24 -3.280 12400.0 / PLOG / 1.20E-01 4.600E+24 -3.380 14700.0 / PLOG / 1.00E+00
2.400E+20 -2.040 15400.0 / C4H5-N=C4H5-I 1.500E+67 -16.890 59100.0 PLOG / 1.32E-02 2.400E+60
-16.080 47500.0 / PLOG / 2.63E-02 1.300E+62 -16.380 49600.0 / PLOG / 1.20E-01 4.900E+66
-17.260 55400.0 / PLOG / 1.00E+00 1.500E+67 -16.890 59100.0 / PLOG / 1.00E+01 2.000E+60
-14.460 58600.0 / C4H4+H=C4H5-N 4.330E+50 -11.920 16500.0 PLOG / 1.32E-02 4.000E+50
-12.570 12300.0 / PLOG / 2.63E-02 1.400E+50 -12.340 12500.0 / PLOG / 1.20E-01 3.670E+49
-11.940 13400.0 / PLOG / 1.00E+00 4.330E+50 -11.920 16500.0 / PLOG / 1.00E+01 2.070E+45
-10.080 15800.0 / C4H4+H=C4H5-I 4.900E+51 -11.920 17700.0 PLOG / 1.32E-02 6.100E+53 -
13.190 14200.0 / PLOG / 2.63E-02 9.600E+52 -12.850 14300.0 / PLOG / 1.20E-01 2.100E+52
-12.440 15500.0 / PLOG / 1.00E+00 4.900E+51 -11.920 17700.0 / PLOG / 1.00E+01 1.500E+48 -
10.580 18800.0 / C4H5-N+H=C4H5-I+H 3.100E+26 -3.350 17423.0 C4H5-N+H=C4H4+H2 1.500E+13
0.000 0.0 C4H5-N+OH=C4H4+H2O 2.000E+12 0.000 0.0 C4H5-N+HCO=C4H6+CO 5.000E+12
0.000 0.0 C4H5-N+HO2=¿C2H3+CH2CO+OH 6.600E+12 0.000 0.0 C4H5-N+O2=CH2CHCHCHO+O
7.360E+12 0.000 1041.0 C4H5-N+O2=¿H+CO+C2H3CHO 4.260E+11 0.000 -1537.0 C4H5-N+O2=HCO+C2H3C
1.830E+11 0.000 -1537.0 C4H5-I+H=C4H4+H2 3.000E+13 0.000 0.0 C4H5-I+H=C3H3+CH3
2.000E+13 0.000 2000.0 C4H5-I+OH=C4H4+H2O 4.000E+12 0.000 0.0 C4H5-I+HCO=C4H6+CO
5.000E+12 0.000 0.0 C4H5-I+HO2=¿C2H3+CH2CO+OH 6.600E+12 0.000 0.0 C4H5-I+O2=CH2CO+CH2CHO
2.160E+10 0.000 2500.0 C4H5-2=C4H5-I 1.500E+67 -16.890 59100.0 C4H5-2+H=C4H5-I+H 3.100E+26
-3.350 17423.0 C4H5-2+HO2=¿OH+C2H2+CH3CO 8.000E+11 0.000 0.0 C4H5-2+O2=CH3CO+CH2CO
2.160E+10 0.000 2500.0 C4H5-2+OH=CH2OH+C3H3 3.000E+12 0.000 0.0 C4H5-2+O=CH2O+C3H3
3.000E+13 0.000 0.0 C4H6+C2H3=¿C6H6+H2+H 5.620E+11 0.000 3240.0 C4H5-I+C2H2=FULVENE+H
9.740E+26 -3.760 21329.0 C4H5-N+C2H2=FULVENE+H 1.740E+19 -1.860 12384.0 C4H5-N+C2H2=C6H6+H
1.600E+16 -1.330 5400.0 C4H5-N+C2H3=C6H6+H2 1.840E-13 7.070 -3611.0 C4H5-2+C2H=C3H3+C3H3
4.000E+12 0.000 0.0 C4H5-2+C2H2=C6H6+H 5.000E+14 0.000 25000.0 C4H5-2+C2H4=C5H6+CH3
5.000E+14 0.000 25000.0 C4H612=C4H5-I+H 4.200E+15 0.000 92600.0 C4H612=C4H6 3.000E+13
0.000 65000.0 C3H3+CH3(+M)=C4H612(+M) 1.500E+12 0.000 0.0 LOW / 2.600E+57 -11.940
9770.0 / TROE / 1.750E-01 1.341E+03 6.000E+04 9.770E+03 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/
CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ C4H612+H=C4H5-I+H2 1.700E+05 2.500 2490.0
C4H612+CH3=C4H5-I+CH4 7.000E+13 0.000 18500.0 C4H612+O=C4H5-I+OH 1.800E+11 0.700
5880.0 C4H612+OH=C4H5-I+H2O 3.100E+06 2.000 -298.0 C4H612+H=C4H6+H 2.000E+13
0.000 4000.0 C4H612+H=C3H4-A+CH3 2.000E+13 0.000 2000.0 C4H612+H=C3H4-P+CH3 2.000E+13
0.000 2000.0 C4H612+O=CH2CO+C2H4 1.200E+08 1.650 327.0 C4H6-2=C4H6 3.000E+13 0.000

65000.0 C4H6-2=C4H612 3.000E+13 0.000 67000.0 C4H6-2+H=C4H612+H 2.000E+13 0.000
4000.0 C4H6-2+H=C4H5-2+H2 3.400E+05 2.500 2490.0 C4H6-2+H=CH3+C3H4-P 2.600E+05
2.500 1000.0 C4H6-2=H+C4H5-2 5.000E+15 0.000 87300.0 C4H6-2+CH3=C4H5-2+CH4 1.400E+14
0.000 18500.0 C4H3-I+H=C4H4 3.400E+43 -9.010 12120.0 C4H4+H=C4H3-N+H2 6.650E+05
2.530 12240.0 C4H4+OH=C4H3-N+H2O 3.100E+07 2.000 3430.0 C4H4+H=C4H3-I+H2 3.330E+05
2.530 9240.0 C4H4+OH=C4H3-I+H2O 1.550E+07 2.000 430.0 C4H4+CH3=C4H3-I+CH4 5.000E+13
0.000 19800.0 C4H4+CH3=C4H3-N+CH4 1.000E+14 0.000 22800.0 C3H3+CH2=C4H4+H 5.000E+13
0.000 0.0 C4H4+O=C3H3+HCO 6.000E+08 1.450 -860.0 C4H4+OH=CH2O+C3H3 5.000E+12
0.000 0.0 C2H2+C2H(+M)=C4H3-N(+M) 8.300E+10 0.899 -363.0 LOW / 1.240E+31 -4.718
1871.0 / TROE / 1.000E+00 1.000E+02 5.613E+03 1.339E+04 / H2/ 2.00/ H2O/ 6.00/ CH4/
2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/ 2.50/ C2H4/ 2.50/ C2H2+C2H(+M)=C4H3-
I(+M) 8.300E+10 0.899 -363.0 LOW / 1.240E+31 -4.718 1871.0 / TROE / 1.000E+00 1.000E+02
5.613E+03 1.339E+04 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/
3.00/ C2H2/ 2.50/ C2H4/ 2.50/ C4H2+H=C4H3-N 1.100E+42 -8.720 15300.0 C4H2+H=C4H3-
I 1.100E+30 -4.920 10800.0 C4H3-N=C4H3-I 4.100E+43 -9.490 53000.0 C4H3-N+H=C4H3-I+H
2.500E+20 -1.670 10800.0 C4H3-N+H=C2H2+H2CC 6.300E+25 -3.340 10014.0 C4H3-N+H=C4H4
2.000E+47 -10.260 13070.0 C4H3-N+H=C4H2+H2 3.000E+13 0.000 0.0 C4H3-N+OH=C4H2+H2O
2.000E+12 0.000 0.0 C4H3-N+C2H3=C3H3+C3H3 4.000E+12 0.000 0.0 C3H3+CH=C4H3-I+H
5.000E+13 0.000 0.0 C4H3-I+H=C2H2+H2CC 2.800E+23 -2.550 10780.0 C4H3-I+H=C4H2+H2
6.000E+13 0.000 0.0 C4H3-I+OH=C4H2+H2O 4.000E+12 0.000 0.0 C4H3-I+O2=HCCO+CH2CO
7.860E+16 -1.800 0.0 C4H3-I+CH2=C3H4-A+C2H 2.000E+13 0.000 0.0 C4H4+C2H=L-C6H4+H
1.200E+13 0.000 0.0 C4H3-N+C2H2=L-C6H4+H 2.500E+14 -0.560 10600.0 C4H3-N+C2H2=C-
C6H4+H 6.900E+46 -10.010 30100.0 C4H3-N+C2H2=C6H5 9.600E+70 -17.770 31300.0 C4H3-
I+CH3=C5H6 1.000E+12 0.000 0.0 C3H3+HCCO=C4H4+CO 2.500E+13 0.000 0.0 H2CC+C2H2(+M)=C4H4(+M
3.500E+05 2.055 -2400.0 LOW / 1.400E+60 -12.599 7417.0 / TROE / 9.800E-01 5.600E+01
5.800E+02 4.164E+03 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/
C2H2/ 3.00/ C2H4/ 3.00/ C2H2+C2H=C4H2+H 9.600E+13 0.000 0.0 C4H2+OH=H2C4O+H
6.600E+12 0.000 -410.0 C4H2+OH=CO+C3H3 2.580E+19 -2.440 3034.0 H2C4O+H=C2H2+HCCO
5.000E+13 0.000 3000.0 H2C4O+OH=CH2CO+HCCO 1.000E+07 2.000 2000.0 C4H2+C2H=C6H2+H
9.600E+13 0.000 0.0 C4H2+C2H=C6H3 4.500E+37 -7.680 7100.0 NC3H7CHO+O2=NC3H7CO+HO2
3.010E+13 0.000 39150.0 NC3H7CHO+O=NC3H7CO+OH 5.940E+12 0.000 1868.0 NC3H7CHO+H=NC3H7CO+
1.310E+05 2.580 1220.0 NC3H7CHO+OH=NC3H7CO+H2O 3.370E+12 0.000 -619.0 NC3H7CHO+HO2=NC3H7C
3.010E+12 0.000 11920.0 NC3H7CHO+CH3=NC3H7CO+CH4 7.080E-04 4.580 1966.0 NC3H7CHO+CH3O2=NC3
3.010E+12 0.000 11920.0 NC3H7CHO+OH=C3H6CHO-3+H2O 5.520E+02 3.120 -1176.0 NC3H7CHO+HO2=C3H
3+H2O2 3.440E+12 0.050 17880.0 NC3H7CHO+CH3O2=C3H6CHO-3+CH3O2H 3.440E+12 0.050
17880.0 NC3H7CHO+OH=C3H6CHO-2+H2O 4.680E+07 1.610 -35.0 NC3H7CHO+HO2=C3H6CHO-

2+H2O2 9.640E+03 2.600 13910.0 NC3H7CHO+CH3O2=C3H6CHO-2+CH3O2H 9.640E+03 2.600
13910.0 NC3H7CHO+OH=C3H6CHO-1+H2O 5.280E+09 0.970 1586.0 NC3H7CHO+HO2=C3H6CHO-
1+H2O2 2.380E+04 2.550 16490.0 NC3H7CHO+CH3O2=C3H6CHO-1+CH3O2H 2.380E+04 2.550
16490.0 NC3H7CO=NC3H7+CO 1.000E+11 0.000 9600.0 C2H5CHCO+H=C3H6CHO-3 5.000E+12
0.000 1200.0 C2H3CHO+CH3=C3H6CHO-3 1.230E+11 0.000 7800.0 C3H6CHO-1=C2H4+CH2CHO
7.400E+11 0.000 21970.0 C2H5CHCO+OH=NC3H7+CO2 3.730E+12 0.000 -1010.0 C2H5CHCO+H=NC3H7+CO
4.400E+12 0.000 1459.0 C2H5CHCO+O=C3H6+CO2 3.200E+12 0.000 -437.0 SC3H5CHO=C3H6+CO
3.900E+14 0.000 69000.0 SC3H5CO+H=SC3H5CHO 1.000E+14 0.000 0.0 CH2CHCHCHO+H=SC3H5CHO
1.000E+14 0.000 0.0 SC3H5CHO+OH=SC3H5CO+H2O 3.370E+12 0.000 -619.0 SC3H5CHO+HO2=SC3H5CO+H
1.000E+12 0.000 11920.0 SC3H5CHO+CH3=SC3H5CO+CH4 3.980E+12 0.000 8700.0 SC3H5CHO+O=SC3H5CO
7.180E+12 0.000 1389.0 SC3H5CHO+O2=SC3H5CO+HO2 4.000E+13 0.000 37600.0 SC3H5CHO+H=SC3H5CO-
2.600E+12 0.000 2600.0 SC3H5CHO+C2H3=SC3H5CO+C2H4 1.110E+00 3.500 4682.0 SC3H5CHO+H=CH2CHC
1.700E+05 2.500 2490.0 SC3H5CHO+O=CH2CHCHCHO+OH 5.240E+11 0.700 5884.0 SC3H5CHO+OH=CH2CH
4.460E+06 2.072 1051.0 SC3H5CHO+CH3=CH2CHCHCHO+CH4 2.100E+00 3.500 5675.0 SC3H5CHO+C2H3=C
2.210E+00 3.500 4682.0 SC3H5CHO+H=CH3+C2H3CHO 4.000E+21 -2.390 11180.0 SC3H5CHO+H=C3H6+HCO
4.000E+21 -2.390 11180.0 C3H5-S+CO=SC3H5CO 5.000E+12 0.000 8000.0 CH2CHCHCHO=C3H5-
A+CO 6.100E+05 0.920 -1120.0 CH2CHCHCHO+O2=C2H3CHO+HOCO 1.200E+36 -7.250 33600.0
C2H3COCH3+OH=CH3CHO+CH3CO 1.000E+11 0.000 0.0 C2H3COCH3+OH=¿CH2CO+C2H3+H2O
5.100E+11 0.000 1192.0 C2H3COCH3+HO2=¿CH2CHO+CH3CO+OH 6.030E+09 0.000 7949.0
C2H3COCH3+HO2=¿CH2CO+C2H3+H2O2 8.500E+12 0.000 20460.0 C2H3COCH3+CH3O2=¿CH2CHO+CH3C
3.970E+11 0.000 17050.0 C2H3COCH3+CH3O2=¿CH2CO+C2H3+CH3O2H 3.010E+12 0.000 17580.0
C2H5COCH3+OH=CH2CH2COCH3+H2O 7.550E+09 0.970 1586.0 C2H5COCH3+HO2=CH2CH2COCH3+H2O2
2.380E+04 2.550 16490.0 C2H5COCH3+O=CH2CH2COCH3+OH 2.250E+13 0.000 7700.0 C2H5COCH3+H=CH2
9.160E+06 2.000 7700.0 C2H5COCH3+O2=CH2CH2COCH3+HO2 2.050E+13 0.000 51310.0 C2H5COCH3+CH3=
3.190E+01 3.170 7172.0 C2H5COCH3+CH3O=CH2CH2COCH3+CH3OH 2.170E+11 0.000 6460.0
C2H5COCH3+CH3O2=CH2CH2COCH3+CH3O2H 3.010E+12 0.000 19380.0 C2H5COCH3+C2H3=CH2CH2COC
5.000E+11 0.000 10400.0 C2H5COCH3+C2H5=CH2CH2COCH3+C2H6 5.000E+10 0.000 13400.0
C2H5COCH3+OH=CH3CHCOCH3+H2O 8.450E+11 0.000 -228.0 C2H5COCH3+HO2=CH3CHCOCH3+H2O2
2.000E+11 0.000 8698.0 C2H5COCH3+O=CH3CHCOCH3+OH 3.070E+13 0.000 3400.0 C2H5COCH3+H=CH3CH
4.460E+06 2.000 3200.0 C2H5COCH3+O2=CH3CHCOCH3+HO2 1.550E+13 0.000 41970.0 C2H5COCH3+CH3=C
1.740E+00 3.460 3680.0 C2H5COCH3+CH3O=CH3CHCOCH3+CH3OH 1.450E+11 0.000 2771.0
C2H5COCH3+CH3O2=CH3CHCOCH3+CH3O2H 2.000E+12 0.000 15250.0 C2H5COCH3+C2H3=CH3CHCOCH3
3.000E+11 0.000 3400.0 C2H5COCH3+C2H5=CH3CHCOCH3+C2H6 3.000E+10 0.000 8600.0
C2H5COCH3+OH=C2H5COCH2+H2O 5.100E+11 0.000 1192.0 C2H5COCH3+HO2=C2H5COCH2+H2O2
2.380E+04 2.550 14690.0 C2H5COCH3+O=C2H5COCH2+OH 5.000E+12 0.000 5962.0 C2H5COCH3+H=C2H5C
9.300E+12 0.000 6357.0 C2H5COCH3+O2=C2H5COCH2+HO2 2.050E+13 0.000 49150.0 C2H5COCH3+CH3=C2

1.620E+11 0.000 9630.0 C2H5COCH3+CH3O=C2H5COCH2+CH3OH 2.170E+11 0.000 4660.0
C2H5COCH3+CH3O2=C2H5COCH2+CH3O2H 3.010E+12 0.000 17580.0 C2H5COCH3+C2H3=C2H5COCH2+C2
6.150E+10 0.000 4278.0 C2H5COCH3+C2H5=C2H5COCH2+C2H6 5.000E+10 0.000 11600.0 C2H3COCH3+H=C
5.000E+12 0.000 1200.0 CH3CHCO+CH3=CH3CHCOCH3 1.230E+11 0.000 7800.0 C2H5COCH2=CH2CO+C2H5
1.000E+14 0.000 35000.0 CH3CHCOCH3+O2=CH3CHOOCOCH3 1.000E+11 0.000 0.0 CH3CHOOCOCH3=CH2C
8.900E+12 0.000 29700.0 C2H3COCH3+HO2=CH2CHOOHCOCH3 7.000E+10 0.000 7800.0 NC5H12=NC3H7+C2
5.200E+24 -2.071 88080.0 PLOG / 1.00E-02 1.180E+96 -23.170 126046.0 / PLOG / 1.00E-01
1.860E+89 -20.900 125630.0 / PLOG / 1.00E+00 3.550E+76 -17.020 120458.0 / PLOG / 2.00E+00
3.480E+71 -15.540 117854.0 / PLOG / 5.00E+00 2.160E+64 -13.430 113815.0 / PLOG / 1.00E+01
4.550E+58 -11.790 110456.0 / PLOG / 2.00E+01 1.020E+53 -10.150 106996.0 / PLOG / 5.00E+01
9.000E+45 -8.130 102538.0 / NC5H12=PC4H9+CH3 1.450E+22 -1.522 89100.0 PLOG / 1.00E-02
7.090E+92 -22.460 126235.0 / PLOG / 1.00E-01 4.830E+86 -20.360 126331.0 / PLOG / 1.00E+00
3.240E+74 -16.630 121640.0 / PLOG / 2.00E+00 4.030E+69 -15.180 119142.0 / PLOG / 5.00E+00
3.000E+62 -13.090 115199.0 / PLOG / 1.00E+01 6.470E+56 -11.440 111875.0 / PLOG / 2.00E+01
1.360E+51 -9.800 108418.0 / PLOG / 5.00E+01 9.740E+43 -7.750 103923.0 / NC5H12=C5H11-
1+H 4.200E+17 -0.390 101180.0 PLOG / 1.00E-02 1.990E+74 -17.750 124798.0 / PLOG / 1.00E-01
5.720E+76 -18.010 131106.0 / PLOG / 1.00E+00 4.420E+72 -16.460 132942.0 / PLOG / 2.00E+00
4.560E+69 -15.520 132148.0 / PLOG / 5.00E+00 2.640E+64 -13.920 130026.0 / PLOG / 1.00E+01
3.800E+59 -12.480 127648.0 / PLOG / 2.00E+01 1.440E+54 -10.890 124707.0 / PLOG / 5.00E+01
3.280E+46 -8.670 120241.0 / NC5H12=C5H11-2+H 2.490E+18 -0.632 97930.0 PLOG / 1.00E-02
6.930E+79 -19.240 125716.0 / PLOG / 1.00E-01 7.690E+79 -18.830 130425.0 / PLOG / 1.00E+00
2.340E+73 -16.630 130412.0 / PLOG / 2.00E+00 5.640E+69 -15.520 129087.0 / PLOG / 5.00E+00
6.770E+63 -13.740 126353.0 / PLOG / 1.00E+01 4.300E+58 -12.210 123622.0 / PLOG / 2.00E+01
1.060E+53 -10.570 120451.0 / PLOG / 5.00E+01 2.500E+45 -8.360 115883.0 / NC5H12=C5H11-
3+H 1.260E+18 -0.633 97930.0 PLOG / 1.00E-02 3.490E+79 -19.240 125716.0 / PLOG / 1.00E-
01 3.880E+79 -18.840 130425.0 / PLOG / 1.00E+00 1.180E+73 -16.630 130412.0 / PLOG /
2.00E+00 2.840E+69 -15.520 129087.0 / PLOG / 5.00E+00 3.410E+63 -13.740 126353.0 / PLOG
/ 1.00E+01 2.170E+58 -12.210 123622.0 / PLOG / 2.00E+01 5.320E+52 -10.570 120451.0 / PLOG
/ 5.00E+01 1.260E+45 -8.360 115883.0 / NC5H12+O2=C5H11-1+HO2 4.200E+13 0.000 52800.0
NC5H12+O=C5H11-1+OH 1.130E+14 0.000 7850.0 NC5H12+H=C5H11-1+H2 3.490E+05 2.690
6450.0 NC5H12+OH=C5H11-1+H2O 2.730E+07 1.813 868.0 NC5H12+HO2=C5H11-1+H2O2
4.080E+01 3.590 17160.0 NC5H12+CH3=C5H11-1+CH4 9.040E-01 3.650 7154.0 NC5H12+CH3O=C5H11-
1+CH3OH 3.000E+11 0.000 7000.0 NC5H12+CH3O2=C5H11-1+CH3O2H 1.390E+00 3.970 18280.0
NC5H12+C2H5=C5H11-1+C2H6 1.000E+11 0.000 13400.0 NC5H12+C2H3=C5H11-1+C2H4 1.000E+12
0.000 18000.0 NC5H12+O2CHO=C5H11-1+HO2CHO 1.390E+00 3.970 18280.0 NC5H12+O2=C5H11-
2+HO2 2.800E+13 0.000 50160.0 NC5H12+O2=C5H11-3+HO2 1.400E+13 0.000 50160.0 NC5H12+O=C5H11-

2+OH 5.620E+13 0.000 5200.0 NC5H12+O=C5H11-3+OH 2.810E+13 0.000 5200.0 NC5H12+H=C5H11-2+H2 2.600E+06 2.400 4471.0 NC5H12+H=C5H11-3+H2 1.300E+06 2.400 4471.0 NC5H12+OH=C5H11-2+H2O 1.410E+10 0.935 505.0 NC5H12+OH=C5H11-3+H2O 5.720E+06 1.811 -1016.0 NC5H12+HO2=C5H11-2+H2O2 1.260E+02 3.370 13720.0 NC5H12+HO2=C5H11-3+H2O2 6.320E+01 3.370 13720.0 NC5H12+CH3=C5H11-2+CH4 1.680E+05 2.133 7574.0 NC5H12+CH3=C5H11-3+CH4 8.400E+04 2.133 7574.0 NC5H12+CH3O=C5H11-2+CH3OH 2.200E+11 0.000 5000.0 NC5H12+CH3O=C5H11-3+CH3OH 1.100E+11 0.000 5000.0 NC5H12+CH3O2=C5H11-2+CH3O2H 2.040E+01 3.580 14810.0 NC5H12+CH3O2=C5H11-3+CH3O2H 1.020E+01 3.580 14810.0 NC5H12+C2H5=C5H11-2+C2H6 1.000E+11 0.000 10400.0 NC5H12+C2H5=C5H11-3+C2H6 5.000E+10 0.000 10400.0 NC5H12+C2H3=C5H11-2+C2H4 8.000E+11 0.000 16800.0 NC5H12+C2H3=C5H11-3+C2H4 4.000E+11 0.000 16800.0 NC5H12+O2CHO=C5H11-2+HO2CHO 2.040E+01 3.580 14810.0 NC5H12+O2CHO=C5H11-3+HO2CHO 1.020E+01 3.580 14810.0 NC5H12+C5H11-1=C5H11-2+NC5H12 1.000E+11 0.000 10400.0 NC5H12+C5H11-1=C5H11-3+NC5H12 5.000E+10 0.000 10400.0 NC5H12+C5H11-2=C5H11-3+NC5H12 5.000E+10 0.000 12300.0 C5H11-1=C2H4+NC3H7 3.240E+12 0.323 28808.0 PLOG / 1.00E-01 4.410E+03 2.192 18827.0 / PLOG / 1.00E+00 8.060E+20 -2.628 29232.0 / PLOG / 1.00E+01 2.170E+28 -4.578 34864.0 / PLOG / 1.00E+02 6.470E+24 -3.383 34388.0 / PLOG / 1.00E+03 2.340E+17 -1.123 31176.0 / C5H11-1=H+C5H10-1 2.040E+10 0.950 33810.0 PLOG / 1.00E-01 3.240E-14 7.022 15354.0 / PLOG / 1.00E+00 5.100E+12 -0.402 29991.0 / PLOG / 1.00E+01 4.070E+27 -4.483 39814.0 / PLOG / 1.00E+02 1.020E+26 -3.794 40806.0 / PLOG / 1.00E+03 6.520E+16 -0.987 36957.0 / C5H11-2=C3H6+C2H5 4.070E+12 0.272 29140.0 PLOG / 1.00E-01 8.540E+25 -4.241 31303.0 / PLOG / 1.00E+00 2.340E+31 -5.581 35992.0 / PLOG / 1.00E+01 4.630E+28 -4.592 36186.0 / PLOG / 1.00E+02 3.770E+20 -2.108 32927.0 / PLOG / 1.00E+03 3.560E+14 -0.301 30124.0 / C5H11-2=C5H10-1+H 2.240E+08 1.517 34750.0 PLOG / 1.00E-01 8.260E+10 -0.118 29715.0 / PLOG / 1.00E+00 6.920E+26 -4.456 39997.0 / PLOG / 1.00E+01 3.810E+29 -4.969 43662.0 / PLOG / 1.00E+02 4.220E+20 -2.160 40523.0 / PLOG / 1.00E+03 5.050E+11 0.526 36461.0 / C5H11-2=C5H10-2+H 2.710E+09 1.193 34514.0 PLOG / 1.00E-01 2.800E+13 -0.833 30423.0 / PLOG / 1.00E+00 9.920E+27 -4.775 39987.0 / PLOG / 1.00E+01 8.500E+29 -5.063 43151.0 / PLOG / 1.00E+02 1.030E+21 -2.275 39953.0 / PLOG / 1.00E+03 3.140E+12 0.287 36068.0 / C5H11-3=C4H8-1+CH3 2.950E+10 0.928 30048.0 PLOG / 1.00E-01 1.310E+16 -1.137 29671.0 / PLOG / 1.00E+00 1.850E+25 -3.643 35787.0 / PLOG / 1.00E+01 1.010E+24 -3.130 36363.0 / PLOG / 1.00E+02 1.980E+16 -0.793 33017.0 / PLOG / 1.00E+03 2.100E+11 0.685 30583.0 / C5H11-3=C5H10-2+H 1.270E+09 1.330 34418.0 PLOG / 1.00E-01 5.120E+06 1.511 29139.0 / PLOG / 1.00E+00 4.070E+22 -2.949 38766.0 / PLOG / 1.00E+01 2.300E+25 -3.569 41777.0 / PLOG / 1.00E+02 8.100E+16 -0.983 38322.0 / PLOG / 1.00E+03 1.210E+10 1.047 35009.0 / C5H11-1+O2=C5H10-1+HO2 8.370E-01 3.590 11960.0 C5H11-2+O2=C5H10-1+HO2 5.350E-01 3.710 9322.0 C5H11-2+O2=C5H10-2+HO2 1.070E+00 3.710 9322.0 C5H11-

3+O2=C5H10-2+HO2 2.140E+00 3.710 9322.0 C5H11-1=C5H11-2 1.150E+01 3.033 15313.0 PLOG / 1.00E-01 1.610E+10 -0.128 16305.0 / PLOG / 1.00E+00 2.880E+17 -2.073 21414.0 / PLOG / 1.00E+01 5.090E+18 -2.284 23337.0 / PLOG / 1.00E+02 1.380E+14 -0.838 21871.0 / PLOG / 1.00E+03 1.600E+08 0.954 19221.0 / C5H11-1=C5H11-3 3.890E-12 6.843 18781.0 PLOG / 1.00E-01 6.080E-15 6.876 11901.0 / PLOG / 1.00E+00 7.680E+07 0.667 25012.0 / PLOG / 1.00E+01 1.260E+19 -2.350 32938.0 / PLOG / 1.00E+02 1.160E+16 -1.256 33072.0 / PLOG / 1.00E+03 6.060E+06 1.570 29120.0 / C5H11-2=C5H11-3 2.750E+10 0.712 41872.0 PLOG / 1.00E-01 4.800E-04 3.725 28298.0 / PLOG / 1.00E+00 3.410E+22 -3.517 42976.0 / PLOG / 1.00E+01 1.570E+32 -6.005 50425.0 / PLOG / 1.00E+02 3.120E+24 -3.514 48305.0 / PLOG / 1.00E+03 1.590E+14 -0.404 43709.0 / C5H11-1+O2=C5H11O2-1 6.860E+16 -1.627 199.0 C5H11-2+O2=C5H11O2-2 3.490E+14 -0.816 -536.0 C5H11-3+O2=C5H11O2-3 3.490E+14 -0.816 -536.0 C5H11-1+HO2=C5H11O-1+OH 9.000E+12 0.000 -1000.0 C5H11-2+HO2=C5H11O-2+OH 9.000E+12 0.000 -1000.0 C5H11-3+HO2=C5H11O-3+OH 9.000E+12 0.000 -1000.0 C5H11-1+CH3O2=C5H11O-1+CH3O 9.000E+12 0.000 -1000.0 C5H11-2+CH3O2=C5H11O-2+CH3O 9.000E+12 0.000 -1000.0 C5H11-3+CH3O2=C5H11O-3+CH3O 9.000E+12 0.000 -1000.0 C5H11-1+C5H11O2-1=C5H11O-1+C5H11O-1 9.000E+12 0.000 -1000.0 C5H11-1+C5H11O2-2=C5H11O-1+C5H11O-2 9.000E+12 0.000 -1000.0 C5H11-1+C5H11O2-3=C5H11O-1+C5H11O-3 9.000E+12 0.000 -1000.0 C5H11-2+C5H11O2-1=C5H11O-2+C5H11O-1 9.000E+12 0.000 -1000.0 C5H11-2+C5H11O2-2=C5H11O-2+C5H11O-2 9.000E+12 0.000 -1000.0 C5H11-2+C5H11O2-3=C5H11O-2+C5H11O-3 9.000E+12 0.000 -1000.0 C5H11-3+C5H11O2-1=C5H11O-3+C5H11O-1 9.000E+12 0.000 -1000.0 C5H11-3+C5H11O2-2=C5H11O-3+C5H11O-2 9.000E+12 0.000 -1000.0 C5H11-3+C5H11O2-3=C5H11O-3+C5H11O-3 9.000E+12 0.000 -1000.0 C5H11O2-1=C5H10OOH1-2 4.010E+08 1.100 30100.0 C5H11O2-1=C5H10OOH1-3 1.360E+07 1.300 18200.0 C5H11O2-1=C5H10OOH1-4 3.720E+06 1.200 16600.0 C5H11O2-1=C5H10OOH1-5 2.940E+05 1.500 19900.0 C5H11O2-2=C5H10OOH2-1 7.290E+08 1.100 33500.0 C5H11O2-2=C5H10OOH2-3 1.720E+09 0.900 29500.0 C5H11O2-2=C5H10OOH2-4 7.030E+10 0.200 19500.0 C5H11O2-2=C5H10OOH2-5 6.170E+05 1.500 20000.0 C5H11O2-3=C5H10OOH3-1 2.880E+07 1.400 20800.0 C5H11O2-3=C5H10OOH3-2 3.430E+09 0.900 30500.0 C5H11O2-1=PC4H9CHO+OH 1.980E+09 1.200 39700.0 C5H11O2-2=NC3H7COCH3+OH 5.300E+09 1.000 38500.0 C5H11O2-3=C2H5COC2H5+OH 5.300E+09 1.000 38500.0 C5H11O2-1=C5H10-1+HO2 3.870E+07 1.580 28500.0 C5H11O2-2=C5H10-1+HO2 3.600E+09 1.130 30100.0 C5H11O2-2=C5H10-2+HO2 5.140E+09 1.010 29362.0 C5H11O2-3=C5H10-2+HO2 7.200E+10 0.730 30883.0 C5H11O2H-1+O2=C5H11O2-1+HO2 3.750E+13 -0.791 33620.0 C5H11O2H-2+O2=C5H11O2-2+HO2 4.380E+13 -0.812 33640.0 C5H11O2H-3+O2=C5H11O2-3+HO2 4.380E+13 -0.812 33640.0 C5H11O2H-1+HO2=C5H11O2-1+H2O2 2.400E+12 0.000 10000.0 C5H11O2H-2+HO2=C5H11O2-2+H2O2 2.400E+12 0.000 10000.0 C5H11O2H-3+HO2=C5H11O2-3+H2O2 2.400E+12 0.000 10000.0 NC5H12+C5H11O2-1=C5H11-1+C5H11O2H-1 1.210E+13 0.000 20430.0 NC5H12+C5H11O2-2=C5H11-

1+C5H11O2H-2 1.210E+13 0.000 20430.0 NC5H12+C5H11O2-3=C5H11-1+C5H11O2H-3 1.210E+13
0.000 20430.0 NC5H12+C5H11O2-1=C5H11-2+C5H11O2H-1 8.060E+12 0.000 17700.0 NC5H12+C5H11O2-
2=C5H11-2+C5H11O2H-2 8.060E+12 0.000 17700.0 NC5H12+C5H11O2-3=C5H11-2+C5H11O2H-
3 8.060E+12 0.000 17700.0 NC5H12+C5H11O2-1=C5H11-3+C5H11O2H-1 4.030E+12 0.000 17700.0
NC5H12+C5H11O2-2=C5H11-3+C5H11O2H-2 4.030E+12 0.000 17700.0 NC5H12+C5H11O2-3=C5H11-
3+C5H11O2H-3 4.030E+12 0.000 17700.0 C5H11O2-1+CH3O2=¿C5H11O-1+CH3O+O2 1.400E+16
-1.610 1860.0 C5H11O2-2+CH3O2=¿C5H11O-2+CH3O+O2 1.400E+16 -1.610 1860.0 C5H11O2-
3+CH3O2=¿C5H11O-3+CH3O+O2 1.400E+16 -1.610 1860.0 C5H11O2-1+C5H11O2-1=¿C5H11O-
1+C5H11O-1+O2 1.400E+16 -1.610 1860.0 C5H11O2-1+C5H11O2-2=¿C5H11O-1+C5H11O-2+O2
1.400E+16 -1.610 1860.0 C5H11O2-1+C5H11O2-3=¿C5H11O-1+C5H11O-3+O2 1.400E+16 -1.610
1860.0 C5H11O2-2+C5H11O2-2=¿C5H11O-2+C5H11O-2+O2 1.400E+16 -1.610 1860.0 C5H11O2-
2+C5H11O2-3=¿C5H11O-2+C5H11O-3+O2 1.400E+16 -1.610 1860.0 C5H11O2-3+C5H11O2-3=¿C5H11O-
3+C5H11O-3+O2 1.400E+16 -1.610 1860.0 C5H11O2-1+CH3O2=¿PC4H9CHO+CH3OH+O2 1.400E+16
-1.610 1860.0 C5H11O2-1+CH3O2=¿NC5H11OH+CH2O+O2 1.400E+16 -1.610 1860.0 C5H11O2-
2+CH3O2=¿NC3H7COCH3+CH3OH+O2 1.400E+16 -1.610 1860.0 C5H11O2-3+CH3O2=¿C2H5COC2H5+CH3O
1.400E+16 -1.610 1860.0 C5H11O2-1+C2H5O2=¿PC4H9CHO+C2H5OH+O2 3.500E+15 -1.610
1860.0 C5H11O2-1+C2H5O2=¿NC5H11OH+CH3CHO+O2 3.500E+15 -1.610 1860.0 C5H11O2-
2+C2H5O2=¿NC3H7COCH3+C2H5OH+O2 3.500E+15 -1.610 1860.0 C5H11O2-3+C2H5O2=¿C2H5COC2H5+C2
3.500E+15 -1.610 1860.0 C5H11O2-1+C5H11O2-1=¿PC4H9CHO+NC5H11OH+O2 3.500E+15 -
1.610 1860.0 C5H11O2H-1=C5H11O-1+OH 7.300E+18 -0.890 45630.0 C5H11O2H-2=C5H11O-
2+OH 4.230E+20 -1.400 45750.0 C5H11O2H-3=C5H11O-3+OH 1.420E+20 -1.340 45690.0 C5H11O2H-
1+OH=¿PC4H9CHO+H2O+OH 2.000E+12 0.000 0.0 C5H11O2H-2+OH=¿NC3H7COCH3+H2O+OH
1.000E+12 0.000 0.0 C5H11O2H-3+OH=¿C2H5COC2H5+H2O+OH 1.000E+12 0.000 0.0 CH2O+PC4H9=C5H11
1 5.000E+10 0.000 3457.0 CH3CHO+NC3H7=C5H11O-2 3.330E+10 0.000 6397.0 C2H5+C2H5CHO=C5H11O-
3 1.670E+10 0.000 6193.0 C5H10OOH1-2=C5H10O1-2+OH 4.670E+12 0.250 12840.0 PLOG /
1.00E-02 3.900E+07 -0.190 1871.0 / PLOG / 1.00E-01 3.120E+15 -2.190 5978.0 / PLOG /
1.00E+00 3.240E+24 -4.480 11337.0 / PLOG / 2.00E+00 7.600E+26 -5.060 12972.0 / PLOG
/ 5.00E+00 1.800E+29 -5.590 14912.0 / PLOG / 1.00E+01 1.520E+30 -5.730 16062.0 / PLOG /
2.00E+01 1.320E+30 -5.570 16802.0 / PLOG / 5.00E+01 2.460E+28 -4.890 17020.0 / PLOG /
1.00E+02 1.150E+26 -4.090 16650.0 / C5H10OOH1-3=C5H10O1-3+OH 1.280E+05 1.830 14460.0
PLOG / 1.00E-02 4.240E+40 -9.570 25269.0 / PLOG / 1.00E-01 2.430E+26 -4.870 21713.0 /
PLOG / 1.00E+00 2.900E+12 -0.480 16944.0 / PLOG / 2.00E+00 3.680E+10 0.110 16258.0
/ PLOG / 5.00E+00 1.710E+09 0.520 15773.0 / PLOG / 1.00E+01 5.610E+08 0.680 15596.0
/ PLOG / 2.00E+01 3.150E+08 0.750 15504.0 / PLOG / 5.00E+01 2.210E+08 0.800 15448.0
/ PLOG / 1.00E+02 1.960E+08 0.820 15429.0 / C5H10OOH1-4=C5H10O1-4+OH 4.730E+05
1.240 8130.0 PLOG / 1.00E-02 1.470E+18 -3.060 10191.0 / PLOG / 1.00E-01 2.800E+14 -1.590

10655.0 / PLOG / 1.00E+00 5.970E+09 -0.070 9377.0 / PLOG / 2.00E+00 2.060E+09 0.080 9236.0 / PLOG / 5.00E+00 1.040E+09 0.180 9144.0 / PLOG / 1.00E+01 8.200E+08 0.210 9112.0 / PLOG / 2.00E+01 7.280E+08 0.230 9096.0 / PLOG / 5.00E+01 6.770E+08 0.240 9086.0 / PLOG / 1.00E+02 6.610E+08 0.240 9083.0 / C5H10OOH1-5=C5H10O1-5+OH 2.310E+04 1.310 8550.0 PLOG / 1.00E-02 1.330E+12 -1.190 10872.0 / PLOG / 1.00E-01 1.860E+08 0.060 9760.0 / PLOG / 1.00E+00 4.680E+07 0.260 9574.0 / PLOG / 2.00E+00 4.320E+07 0.270 9563.0 / PLOG / 5.00E+00 4.110E+07 0.270 9556.0 / PLOG / 1.00E+01 4.040E+07 0.280 9554.0 / PLOG / 2.00E+01 4.010E+07 0.280 9553.0 / PLOG / 5.00E+01 3.990E+07 0.280 9552.0 / PLOG / 1.00E+02 3.980E+07 0.280 9552.0 / C5H10OOH2-1=C5H10O1-2+OH 2.570E+09 1.040 11340.0 PLOG / 1.00E-02 2.800E+05 0.520 1289.0 / PLOG / 1.00E-01 6.620E+15 -2.200 6879.0 / PLOG / 1.00E+00 1.950E+25 -4.600 13023.0 / PLOG / 2.00E+00 4.990E+26 -4.880 14402.0 / PLOG / 5.00E+00 5.550E+26 -4.710 15465.0 / PLOG / 1.00E+01 2.070E+25 -4.160 15596.0 / PLOG / 2.00E+01 8.130E+22 -3.330 15213.0 / PLOG / 5.00E+01 1.540E+19 -2.100 14271.0 / PLOG / 1.00E+02 5.360E+16 -1.310 13545.0 / C5H10OOH2-3=C5H10O2-3+OH 4.660E+08 1.090 9850.0 PLOG / 1.00E-02 7.380E-02 2.490 -1612.0 / PLOG / 1.00E-01 2.870E+09 -0.290 4045.0 / PLOG / 1.00E+00 2.110E+18 -2.510 9989.0 / PLOG / 2.00E+00 7.990E+18 -2.550 11002.0 / PLOG / 5.00E+00 3.740E+17 -1.980 11395.0 / PLOG / 1.00E+01 2.230E+15 -1.210 11062.0 / PLOG / 2.00E+01 5.530E+12 -0.350 10430.0 / PLOG / 5.00E+01 5.710E+09 0.620 9572.0 / PLOG / 1.00E+02 1.690E+08 1.110 9099.0 / DUP C5H10OOH2-3=C5H10O2-3+OH 7.460E+08 0.700 9270.0 PLOG / 1.00E-02 8.820E+02 1.330 904.0 / PLOG / 1.00E-01 4.380E+12 -1.160 6812.0 / PLOG / 1.00E+00 5.110E+13 -1.080 9522.0 / PLOG / 2.00E+00 1.050E+12 -0.480 9319.0 / PLOG / 5.00E+00 4.760E+09 0.300 8791.0 / PLOG / 1.00E+01 2.170E+08 0.740 8430.0 / PLOG / 2.00E+01 2.920E+07 1.020 8181.0 / PLOG / 5.00E+01 7.120E+06 1.220 8001.0 / PLOG / 1.00E+02 4.260E+06 1.290 7934.0 / DUP C5H10OOH2-4=C5H10O2-4+OH 3.840E+06 1.260 14970.0 PLOG / 1.00E-02 1.570E+32 -7.030 22485.0 / PLOG / 1.00E-01 2.910E+16 -1.950 17872.0 / PLOG / 1.00E+00 3.480E+06 1.170 14400.0 / PLOG / 2.00E+00 3.330E+05 1.480 14031.0 / PLOG / 5.00E+00 7.180E+04 1.690 13788.0 / PLOG / 1.00E+01 4.200E+04 1.760 13704.0 / PLOG / 2.00E+01 3.200E+04 1.800 13660.0 / PLOG / 5.00E+01 2.710E+04 1.820 13634.0 / PLOG / 1.00E+02 2.570E+04 1.830 13625.0 / DUP C5H10OOH2-4=C5H10O2-4+OH 1.390E+06 1.490 15210.0 PLOG / 1.00E-02 1.140E+36 -8.190 23953.0 / PLOG / 1.00E-01 2.240E+20 -3.080 19618.0 / PLOG / 1.00E+00 2.860E+07 0.970 15137.0 / PLOG / 2.00E+00 7.110E+05 1.470 14555.0 / PLOG / 5.00E+00 5.640E+04 1.820 14153.0 / PLOG / 1.00E+01 2.270E+04 1.940 14008.0 / PLOG / 2.00E+01 1.420E+04 2.000 13933.0 / PLOG / 5.00E+01 1.070E+04 2.040 13887.0 / PLOG / 1.00E+02 9.710E+03 2.060 13872.0 / DUP C5H10OOH2-5=C5H10O1-4+OH 3.780E+05 1.280 10220.0 PLOG / 1.00E-02 2.520E+20 -3.620 13849.0 / PLOG / 1.00E-01 1.090E+12 -0.820 11988.0 / PLOG / 1.00E+00 9.190E+07 0.480 10691.0 /

PLOG / 2.00E+00 4.390E+07 0.580 10585.0 / PLOG / 5.00E+00 2.770E+07 0.640 10518.0 / PLOG / 1.00E+01 2.370E+07 0.660 10496.0 / PLOG / 2.00E+01 2.190E+07 0.670 10484.0 / PLOG / 5.00E+01 2.090E+07 0.680 10477.0 / PLOG / 1.00E+02 2.060E+07 0.680 10475.0 / C5H10OOH3-1=C5H10O1-3+OH 2.400E+06 1.520 17240.0 PLOG / 1.00E-02 2.630E+42 -9.990 28572.0 / PLOG / 1.00E-01 4.280E+25 -4.560 23726.0 / PLOG / 1.00E+00 1.020E+12 -0.290 18930.0 / PLOG / 2.00E+00 1.760E+10 0.260 18283.0 / PLOG / 5.00E+00 1.040E+09 0.640 17830.0 / PLOG / 1.00E+01 3.750E+08 0.780 17665.0 / PLOG / 2.00E+01 2.210E+08 0.850 17580.0 / PLOG / 5.00E+01 1.600E+08 0.900 17528.0 / PLOG / 1.00E+02 1.430E+08 0.910 17510.0 / C5H10OOH3-2=C5H10O2-3+OH 2.810E+09 0.350 9860.0 PLOG / 1.00E-02 7.370E+08 -0.390 4687.0 / PLOG / 1.00E-01 3.620E+14 -1.670 9295.0 / PLOG / 1.00E+00 5.600E+10 -0.220 9449.0 / PLOG / 2.00E+00 2.080E+09 0.250 9104.0 / PLOG / 5.00E+00 1.180E+08 0.660 8769.0 / PLOG / 1.00E+01 3.610E+07 0.830 8623.0 / PLOG / 2.00E+01 1.880E+07 0.920 8542.0 / PLOG / 5.00E+01 1.250E+07 0.980 8490.0 / PLOG / 1.00E+02 1.080E+07 1.000 8472.0 / DUP C5H10OOH3-2=C5H10O2-3+OH 4.200E+09 0.710 10050.0 PLOG / 1.00E-02 1.570E+00 2.100 -841.0 / PLOG / 1.00E-01 3.250E+10 -0.590 4837.0 / PLOG / 1.00E+00 3.930E+17 -2.280 10081.0 / PLOG / 2.00E+00 3.220E+17 -2.120 10773.0 / PLOG / 5.00E+00 4.630E+15 -1.420 10845.0 / PLOG / 1.00E+01 3.340E+13 -0.690 10443.0 / PLOG / 2.00E+01 2.470E+11 0.010 9905.0 / PLOG / 5.00E+01 1.910E+09 0.690 9301.0 / PLOG / 1.00E+02 2.070E+08 1.000 9009.0 / DUP C5H10OOH1-2=C5H10-1+HO2 1.040E+10 0.940 15100.0 C5H10OOH2-1=C5H10-1+HO2 2.210E+12 0.230 15600.0 C5H10OOH2-3=C5H10-2+HO2 4.540E+10 0.751 15100.0 C5H10OOH3-2=C5H10-2+HO2 4.070E+10 0.678 15034.0 C5H10OOH1-3=¿OH+CH2O+C4H8-1 9.100E+08 1.400 25500.0 C5H10OOH2-4=¿OH+CH3CHO+C3H6 1.180E+09 1.200 22700.0 C5H10OOH3-1=¿OH+C2H5CHO+C2H4 3.100E+18 -1.730 26820.0 C5H10OOH1-2=C2H5+AC3H5OOH 2.410E+10 1.020 28200.0 C5H10OOH1-4=C3H6+C2H4O2H 5.080E+11 0.700 28700.0 C5H10OOH2-5=C2H4+C3H6OOH2-1 6.860E+13 0.100 29000.0 C5H10OOH1-2+O2=C5H10OOH1-2O2 1.570E+14 -0.816 -536.0 C5H10OOH1-3+O2=C5H10OOH1-3O2 1.570E+14 -0.816 -536.0 C5H10OOH1-4+O2=C5H10OOH1-4O2 1.570E+14 -0.816 -536.0 C5H10OOH1-5+O2=C5H10OOH1-5O2 3.090E+16 -1.627 199.0 C5H10OOH2-1+O2=C5H10OOH2-1O2 3.090E+16 -1.627 199.0 C5H10OOH2-3+O2=C5H10OOH2-3O2 1.570E+14 -0.816 -536.0 C5H10OOH2-4+O2=C5H10OOH2-4O2 1.570E+14 -0.816 -536.0 C5H10OOH2-5+O2=C5H10OOH2-5O2 3.090E+16 -1.627 199.0 C5H10OOH3-1+O2=C5H10OOH3-1O2 3.090E+16 -1.627 199.0 C5H10OOH3-2+O2=C5H10OOH3-2O2 1.570E+14 -0.816 -536.0 C5H10OOH1-2O2=C5H92-1OOH+HO2 5.140E+09 1.010 29362.0 C5H10OOH1-3O2=C5H92-1OOH+HO2 3.600E+10 0.730 29883.0 C5H10OOH1-3O2=C5H92-5OOH+HO2 3.600E+10 0.730 29883.0 C5H10OOH1-4O2=C5H91-5OOH+HO2 3.600E+09 1.130 30100.0 C5H10OOH1-4O2=C5H92-5OOH+HO2 5.140E+09 1.010 29362.0 C5H10OOH1-5O2=C5H91-5OOH+HO2 3.870E+07 1.580 28500.0 C5H10OOH2-3O2=C5H92-4OOH+HO2 3.600E+10 0.730 29883.0 C5H10OOH2-4O2=C5H92-4OOH+HO2 5.140E+09 1.010 29362.0 C5H10OOH2-

4O2=C5H91-4OOH+HO2 3.600E+09 1.130 30100.0 C5H10OOH2-5O2=C5H91-4OOH+HO2 3.870E+07 1.580 28500.0 C5H10OOH3-1O2=C5H91-3OOH+HO2 3.870E+07 1.580 28500.0 C5H10OOH3-2O2=C5H91-3OOH+HO2 3.600E+09 1.130 30100.0 C5H10OOH1-2O2=C5H93-1,2OOH 1.720E+09 0.900 29500.0 C5H10OOH1-2O2=C5H92-4,5OOH 7.030E+10 0.200 18500.0 C5H10OOH1-2O2=C5H91-4,5OOH 1.230E+06 1.500 20000.0 C5H10OOH1-3O2=C5H92-1,3OOH 3.430E+09 0.900 29500.0 C5H10OOH1-3O2=C5H92-3,5OOH 3.430E+09 0.900 29500.0 C5H10OOH1-3O2=C5H91-3,5OOH 2.880E+07 1.400 20800.0 C5H10OOH1-4O2=C5H92-1,4OOH 7.030E+10 0.200 18500.0 C5H10OOH1-4O2=C5H93-1,4OOH 1.720E+09 0.900 29500.0 C5H10OOH1-4O2=C5H91-2,5OOH 7.290E+08 1.100 33500.0 C5H10OOH1-5O2=C5H92-1,5OOH 3.720E+06 1.200 16600.0 DUP C5H10OOH1-5O2=C5H93-1,5OOH 1.360E+07 1.300 18200.0 C5H10OOH1-5O2=C5H92-1,5OOH 4.010E+08 1.100 30100.0 DUP C5H10OOH2-1O2=C5H93-1,2OOH 1.360E+07 1.300 18200.0 C5H10OOH2-1O2=C5H92-4,5OOH 3.720E+06 1.200 16600.0 C5H10OOH2-1O2=C5H91-4,5OOH 2.940E+05 1.500 19900.0 C5H10OOH2-3O2=C5H91-2,3OOH 2.880E+07 1.400 20800.0 C5H10OOH2-3O2=C5H92-3,4OOH 3.430E+09 0.900 29500.0 C5H10OOH2-3O2=C5H91-3,4OOH 2.880E+07 1.400 20800.0 C5H10OOH2-4O2=C5H91-2,4OOH 1.230E+06 1.500 20000.0 DUP C5H10OOH2-4O2=C5H93-2,4OOH 1.720E+09 0.900 29500.0 C5H10OOH2-4O2=C5H91-2,4OOH 7.290E+08 1.100 33500.0 DUP C5H10OOH2-5O2=C5H91-2,5OOH 2.940E+05 1.500 19900.0 C5H10OOH2-5O2=C5H93-1,4OOH 1.360E+07 1.300 18200.0 C5H10OOH2-5O2=C5H92-1,4OOH 4.010E+08 1.100 30100.0 C5H10OOH3-1O2=C5H92-1,3OOH 4.010E+08 1.100 30100.0 C5H10OOH3-1O2=C5H92-3,5OOH 3.720E+06 1.200 16600.0 C5H10OOH3-1O2=C5H91-3,5OOH 2.940E+05 1.500 19900.0 C5H10OOH3-2O2=C5H91-2,3OOH 7.290E+08 1.100 33500.0 C5H10OOH3-2O2=C5H92-3,4OOH 7.030E+10 0.200 18500.0 C5H10OOH3-2O2=C5H91-3,4OOH 1.230E+06 1.500 20000.0 C5H10OOH1-2O2=NC5KET12+OH 2.440E+07 1.600 27900.0 C5H10OOH1-3O2=NC5KET13+OH 1.100E+04 2.400 19900.0 C5H10OOH1-4O2=NC5KET14+OH 1.260E+03 2.200 17400.0 C5H10OOH1-5O2=NC5KET15+OH 1.120E+03 1.800 16600.0 C5H10OOH2-1O2=NC5KET21+OH 2.760E+08 1.200 25700.0 C5H10OOH2-3O2=NC5KET23+OH 1.750E+08 1.700 26000.0 C5H10OOH2-4O2=NC5KET24+OH 1.750E+02 3.100 17500.0 C5H10OOH2-5O2=NC5KET25+OH 3.770E+02 2.200 15300.0 C5H10OOH3-1O2=NC5KET31+OH 5.790E+01 2.900 17000.0 C5H10OOH3-2O2=NC5KET32+OH 1.750E+08 1.700 26000.0 C5H10OOH1-3O2+C5H10OOH1-3O2=¿NC5KET31+C5H10OOH3OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH1-3O2+C5H10OOH2-4O2=¿NC5KET31+C5H10OOH2-4OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH1-3O2+C5H10OOH2-4O2=¿NC5KET24+C5H10OOH1-3OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH1-3O2+C5H10OOH3-1O2=¿NC5KET31+C5H10OOH3-1OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH1-3O2+C5H10OOH3-1O2=¿NC5KET13+C5H10OOH1-3OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH2-4O2+C5H10OOH2-4O2=¿NC5KET24+C5H10OOH2-4OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH2-4O2+C5H10OOH3-1O2=¿NC5KET24+C5H10OOH3-1OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH2-4O2+C5H10OOH3-1O2=¿NC5KET13+C5H10OOH2-4OH+O2 1.400E+16 -1.610 1860.0 C5H10OOH3-1O2+C5H10OOH3-1O2=¿NC5KET13+C5H10OOH3-

1OH+O2 1.400E+16 -1.610 1860.0 C5H91-3,4OOH=¿C3KET12+C2H4+OH 3.100E+18 -1.730
26820.0 C5H91-3,5OOH=¿C3KET13+C2H4+OH 3.100E+18 -1.730 26820.0 C5H91-4,5OOH=¿AC3H5OOH+C2H4
6.860E+13 0.100 29000.0 C5H92-1,4OOH=¿AC3H5OOH+CH3CHO+OH 2.410E+10 1.020 28200.0
C5H92-1,5OOH=AC3H5OOH+C2H4O2H 2.410E+10 1.020 28200.0 C5H92-4,5OOH=¿HO2CH2CHO+C3H6+OH
1.180E+09 1.200 22700.0 C5H93-1,4OOH=¿CH2O+C4H71-3OOH+OH 9.100E+08 1.400 25500.0
C5H93-1,5OOH=¿CH2O+C4H71-4OOH+OH 1.820E+09 1.400 25500.0 NC5KET12=NC5KET12O+OH
1.050E+16 0.000 42600.0 NC5KET13=NC5KET13O+OH 1.050E+16 0.000 42600.0 NC5KET14=NC5KET14O+O
1.050E+16 0.000 42600.0 NC5KET15=NC5KET15O+OH 1.500E+16 0.000 43000.0 NC5KET21=NC5KET21O+O
1.500E+16 0.000 43000.0 NC5KET23=NC5KET23O+OH 1.050E+16 0.000 42600.0 NC5KET24=NC5KET24O+O
1.050E+16 0.000 42600.0 NC5KET25=NC5KET25O+OH 1.500E+16 0.000 43000.0 NC5KET31=NC5KET31O+O
1.500E+16 0.000 43000.0 NC5KET32=NC5KET32O+OH 1.050E+16 0.000 42600.0 NC5KET12O=NC3H7CHO+H
2.900E+12 0.380 11080.0 NC5KET13O=C2H5CHO+CH2CHO 2.900E+12 0.380 11080.0 NC5KET14O=CH3CHO+
2.900E+12 0.380 11080.0 NC5KET15O=CH2O+C3H6CHO-1 2.900E+12 0.380 11080.0 NC5KET21O=CH2O+NC
2.900E+12 0.380 11080.0 NC5KET23O=C2H5CHO+CH3CO 2.900E+12 0.380 11080.0 NC5KET24O=CH3CHO+C
2.900E+12 0.380 11080.0 NC5KET25O=CH2O+CH2CH2COCH3 2.900E+12 0.380 11080.0 NC5KET31O=C2H5C
2.900E+12 0.380 11080.0 NC5KET32O=CH3CHO+C2H5CO 2.900E+12 0.380 11080.0 NC5KET13=NC5CYCPER
2.100E+08 0.000 28000.0 NC5KET24=NC5CYCPER24 2.100E+08 0.000 28000.0 NC5KET31=NC5CYCPER31
2.100E+08 0.000 28000.0 NC5CYCPER13=HOCHO+C2H5COCH3 3.400E+13 0.000 34400.0 NC5CYCPER13=CH
3.700E+13 0.000 36800.0 NC5CYCPER24=CH3COOH+CH3COCH3 3.400E+13 0.000 34400.0
NC5CYCPER31=C2H5COOH+CH3CHO 3.400E+13 0.000 34400.0 C5H10OOH1-3OH=¿CH2O+SC4H8OH-
1+OH 1.000E+16 0.000 43000.0 C5H10OOH2-4OH=¿CH3CHO+C3H6OH2-1+OH 1.000E+16 0.000
43000.0 C5H10OOH3-1OH=¿C2H5CHO+PC2H4OH+OH 1.000E+16 0.000 43000.0 NC5KET13+OH=¿NC5DION
1.000E+12 0.000 0.0 NC5KET24+OH=¿NC5DIONE24+OH+H2O 1.000E+12 0.000 0.0 NC5KET31+OH=¿NC5D
2.000E+12 0.000 0.0 C5H91-2,3OOH=C5H91-3OOH+HO2 2.210E+12 0.230 15600.0 C5H91-2,4OOH=C5H91-
4OOH+HO2 2.210E+12 0.230 15600.0 C5H91-2,5OOH=C5H91-5OOH+HO2 2.210E+12 0.230
15600.0 C5H92-1,3OOH=C5H91-3OOH+HO2 1.040E+10 0.940 15100.0 C5H92-1,3OOH=C5H92-
1OOH+HO2 4.070E+10 0.678 15034.0 C5H92-1,4OOH=C5H91-4OOH+HO2 1.040E+10 0.940
15100.0 C5H92-1,5OOH=C5H91-5OOH+HO2 1.040E+10 0.940 15100.0 C5H92-3,4OOH=C5H92-
4OOH+HO2 4.070E+10 0.678 15034.0 C5H92-3,5OOH=C5H92-5OOH+HO2 4.070E+10 0.678
15034.0 C5H93-1,2OOH=C5H92-1OOH+HO2 4.540E+10 0.751 15100.0 C5H93-1,4OOH=C5H92-
5OOH+HO2 4.540E+10 0.751 15100.0 C5H93-2,4OOH=C5H92-4OOH+HO2 9.090E+10 0.751
15100.0 C5H91-3OOH=¿C2H5CHO+C2H3+OH 1.050E+16 0.000 41600.0 C5H91-3OOH=¿C2H3CHO+C2H5+OH
1.050E+16 0.000 41600.0 C5H91-4OOH=¿CH3CHO+C3H5-A+OH 1.050E+16 0.000 41600.0 C5H91-
4OOH=¿SC3H5CHO+CH3+OH 1.050E+16 0.000 41600.0 C5H91-5OOH=¿CH2O+C4H71-4+OH
1.500E+16 0.000 42000.0 C5H92-1OOH=¿CH2O+C4H71-1+OH 1.500E+16 0.000 42000.0 C5H92-
4OOH=¿CH3CHO+C3H5-S+OH 1.050E+16 0.000 41600.0 C5H92-4OOH=¿SC3H5CHO+CH3+OH

1.050E+16 0.000 41600.0 C5H92-5OOH=¿CH2O+C4H71-3+OH 1.500E+16 0.000 42000.0 C5H91-2,3OOH=C5H9O1-2OOH-3+OH 5.800E+10 0.430 10700.0 C5H91-2,3OOH=C5H9O1-3OOH-2+OH 1.020E+10 0.460 17700.0 C5H91-2,4OOH=C5H9O1-2OOH-4+OH 5.800E+10 0.430 10700.0 C5H91-2,4OOH=C5H9O1-4OOH-2+OH 1.240E+09 0.350 11200.0 C5H91-2,5OOH=C5H9O1-2OOH-5+OH 5.800E+10 0.430 10700.0 C5H91-2,5OOH=C5H9O1-5OOH-2+OH 1.440E+07 0.760 11300.0 C5H91-3,4OOH=C5H9O1-3OOH-4+OH 1.020E+10 0.460 17700.0 C5H91-3,4OOH=C5H9O1-4OOH-3+OH 1.240E+09 0.350 11200.0 C5H91-3,5OOH=C5H9O1-3OOH-5+OH 1.020E+10 0.460 17700.0 C5H91-3,5OOH=C5H9O1-5OOH-3+OH 1.440E+07 0.760 11300.0 C5H91-4,5OOH=C5H9O1-4OOH-5+OH 1.240E+09 0.350 11200.0 C5H91-4,5OOH=C5H9O1-5OOH-2+OH 1.440E+07 0.760 11300.0 C5H92-1,3OOH=C5H9O1-2OOH-3+OH 3.670E+09 0.930 10900.0 C5H92-1,3OOH=C5H9O2-3OOH-1+OH 7.040E+09 0.784 9591.0 C5H92-1,4OOH=C5H9O1-2OOH-4+OH 3.670E+09 0.930 10900.0 C5H92-1,4OOH=C5H9O2-4OOH-1+OH 1.340E+09 0.700 16415.0 C5H92-1,5OOH=C5H9O1-2OOH-5+OH 3.670E+09 0.930 10900.0 C5H92-1,5OOH=C5H9O1-4OOH-5+OH 2.410E+07 0.940 10000.0 C5H92-3,4OOH=C5H9O2-3OOH-4+OH 7.040E+09 0.784 9591.0 C5H92-3,4OOH=C5H9O2-4OOH-3+OH 1.340E+09 0.700 16415.0 C5H92-3,5OOH=C5H9O2-3OOH-5+OH 7.040E+09 0.784 9591.0 C5H92-3,5OOH=C5H9O1-4OOH-3+OH 2.410E+07 0.940 10000.0 C5H92-4,5OOH=C5H9O2-4OOH-1+OH 1.340E+09 0.700 16415.0 C5H92-4,5OOH=C5H9O1-4OOH-2+OH 2.410E+07 0.940 10000.0 C5H93-1,2OOH=C5H9O1-3OOH-2+OH 4.220E+08 0.900 15300.0 C5H93-1,2OOH=C5H9O2-3OOH-1+OH 2.440E+09 0.900 9403.0 C5H93-1,4OOH=C5H9O1-3OOH-4+OH 4.220E+08 0.900 15300.0 C5H93-1,4OOH=C5H9O2-3OOH-5+OH 2.440E+09 0.900 9403.0 C5H93-1,5OOH=C5H9O1-3OOH-5+OH 4.220E+08 0.900 15300.0 C5H93-2,4OOH=C5H9O2-3OOH-4+OH 4.880E+09 0.900 9403.0 C5H9O1-2OOH-3=¿C2H5CHO+CH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-3OOH-2=¿C2H5CHO+CH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-3OOH-2=¿CH2O+C3H6CHO-3+OH 1.050E+16 0.000 41600.0 C5H9O1-2OOH-4=¿CH3CHO+C3H5O+OH 1.050E+16 0.000 41600.0 C5H9O1-4OOH-2=¿CH2O+C3H6CHO-2+OH 1.050E+16 0.000 41600.0 C5H9O1-4OOH-2=¿C3H6+OCH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-2OOH-5=C5H9O1-2O-5+OH 4.150E+19 -1.310 45700.0 C5H9O1-5OOH-2=¿CH2O+C3H6CHO-1+OH 1.050E+16 0.000 41600.0 C5H9O1-5OOH-2=¿C2H4+CH2OCH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-3OOH-4=¿CH3CHO+CH2CH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-4OOH-3=¿C2H4+C2H4OCHO+OH 1.050E+16 0.000 41600.0 C5H9O1-3OOH-5=¿CH2O+C4H7O1-4+OH 1.500E+16 0.000 42000.0 C5H9O1-5OOH-3=CH2CH2OCH2CH2CHO+OH 1.050E+16 0.000 41600.0 C5H9O1-4OOH-5=¿CH2O+C3H6CHO-1+OH 1.500E+16 0.000 42000.0 C5H9O2-3OOH-1=¿CH2O+C3H6CHO-3+OH 1.500E+16 0.000 42000.0 C5H9O2-4OOH-1=¿CH2O+C3H6CHO-2+OH 1.500E+16 0.000 42000.0 C5H9O2-4OOH-3=¿CH3CHO+CH3CHCHO+OH 1.050E+16 0.000 41600.0 C5H9O2-3OOH-5=¿CH2O+C4H71-O+OH 1.500E+16 0.000 42000.0 C5H10O1-2+OH=¿CH2CO+NC3H7+H2O 2.260E+03 2.730 -4689.0 C5H10O1-3+OH=¿C2H4+C2H5CO+H2O 2.260E+03 2.730 -4689.0 C5H10O1-4+OH=¿CH3COCH2+C2H4+H2O 2.260E+03 2.730 -4689.0 C5H10O1-5+OH=¿CH2CH2CHO+C2H4+H2O

2.260E+03 2.730 -4689.0 C5H10O2-3+OH=¿CH3CHCO+C2H5+H2O 2.260E+03 2.730 -4689.0
C5H10O2-4+OH=¿CH3CO+C3H6+H2O 2.260E+03 2.730 -4689.0 C5H10O1-2+OH=¿C2H3CHO+C2H5+H2O
2.260E+03 2.730 -4689.0 C5H10O1-3+OH=¿HCO+C4H8-1+H2O 2.260E+03 2.730 -4689.0 C5H10O1-
4+OH=¿CH2CHO+C3H6+H2O 2.260E+03 2.730 -4689.0 C5H10O1-5+OH=¿CH2O+C4H71-3+H2O
2.260E+03 2.730 -4689.0 C5H10O2-3+OH=¿C2H3COCH3+CH3+H2O 2.260E+03 2.730 -4689.0
C5H10O2-4+OH=¿CH3CHO+C3H5-S+H2O 2.260E+03 2.730 -4689.0 C5H10O1-2+HO2=¿CH2CO+NC3H7+H2
1.720E+01 3.460 9733.0 C5H10O1-3+HO2=¿C2H4+C2H5CO+H2O2 1.720E+01 3.460 9733.0
C5H10O1-4+HO2=¿CH3COCH2+C2H4+H2O2 1.720E+01 3.460 9733.0 C5H10O1-5+HO2=¿CH2CH2CHO+C2H
1.720E+01 3.460 9733.0 C5H10O2-3+HO2=¿CH3CHCO+C2H5+H2O2 1.720E+01 3.460 9733.0
C5H10O2-4+HO2=¿CH3CO+C3H6+H2O2 1.720E+01 3.460 9733.0 C5H10O1-2+HO2=¿C2H3CHO+C2H5+H2O
1.720E+01 3.460 9733.0 C5H10O1-3+HO2=¿HCO+C4H8-1+H2O2 1.720E+01 3.460 9733.0 C5H10O1-
4+HO2=¿CH2CHO+C3H6+H2O2 1.720E+01 3.460 9733.0 C5H10O1-5+HO2=¿CH2O+C4H71-
3+H2O2 1.720E+01 3.460 9733.0 C5H10O2-3+HO2=¿C2H3COCH3+CH3+H2O2 1.720E+01 3.460
9733.0 C5H10O2-4+HO2=¿CH3CHO+C3H5-S+H2O2 1.720E+01 3.460 9733.0 C5H81-3+OH=CH2O+C4H71-
3 1.000E+12 0.000 0.0 C5H81-3+OH=C2H3CHO+C2H5 1.000E+12 0.000 0.0 C5H81-3+OH=CH3CHO+C3H5-
S 1.000E+12 0.000 0.0 OCH2CHO=CH2O+HCO 2.900E+12 0.380 11080.0 C5H9O1-2O-5=¿CH2O+CH2CHO+C2
1.330E+21 -2.349 25084.0 CH2OCH2CHO=CH2O+CH2CHO 1.600E+13 0.000 25500.0 C2H4OCHO=CH3CHO+H
2.900E+12 0.380 11080.0 C4H7O1-4=CH2O+C3H5-A 1.330E+21 -2.349 25084.0 CH2CH2OCH2CH2CHO=¿CH2O
1.600E+13 0.000 25500.0 NC5DIONE13+OH=¿CH3CHCO+CH2CHO+H2O 2.360E+02 3.150 3050.0
NC5DIONE24+OH=¿CH2CO+CH3COCH2+H2O 1.720E+05 2.400 815.0 IC5H12=IC3H7+C2H5
1.470E+26 -2.659 86860.0 PLOG / 1.00E-02 4.070E+95 -23.370 121614.0 / PLOG / 1.00E-
01 2.800E+90 -21.550 122339.0 / PLOG / 1.00E+00 8.580E+79 -18.270 119001.0 / PLOG /
2.00E+00 3.960E+75 -16.970 117015.0 / PLOG / 5.00E+00 1.410E+69 -15.060 113723.0 / PLOG
/ 1.00E+01 7.290E+63 -13.510 110811.0 / PLOG / 2.00E+01 2.460E+58 -11.910 107645.0 /
PLOG / 5.00E+01 1.550E+51 -9.830 103292.0 / IC5H12=SC4H9+CH3 8.690E+23 -2.019 87290.0
PLOG / 1.00E-02 1.050E+93 -22.640 121641.0 / PLOG / 1.00E-01 1.310E+88 -20.890 122563.0 /
PLOG / 1.00E+00 6.800E+77 -17.670 119420.0 / PLOG / 2.00E+00 3.550E+73 -16.390 117484.0 /
PLOG / 5.00E+00 1.430E+67 -14.490 114248.0 / PLOG / 1.00E+01 7.810E+61 -12.940 111365.0 /
PLOG / 2.00E+01 2.700E+56 -11.350 108218.0 / PLOG / 5.00E+01 1.660E+49 -9.260 103871.0 /
IC5H12=IC4H9+CH3 1.070E+21 -1.460 89070.0 PLOG / 1.00E-02 2.910E+88 -21.680 121666.0 /
PLOG / 1.00E-01 4.790E+84 -20.230 123421.0 / PLOG / 1.00E+00 2.450E+75 -17.280 121108.0 /
PLOG / 2.00E+00 2.210E+71 -16.050 119391.0 / PLOG / 5.00E+00 1.560E+65 -14.220 116397.0 /
PLOG / 1.00E+01 1.120E+60 -12.700 113651.0 / PLOG / 2.00E+01 4.350E+54 -11.120 110591.0 /
PLOG / 5.00E+01 2.490E+47 -9.020 106282.0 / IC5H12=AC5H11+H 5.090E+17 -0.417 101180.0
PLOG / 1.00E-02 8.010E+67 -16.140 118712.0 / PLOG / 1.00E-01 1.480E+72 -16.920 125626.0 /
PLOG / 1.00E+00 7.250E+70 -16.140 129319.0 / PLOG / 2.00E+00 9.570E+68 -15.500 129394.0

/ PLOG / 5.00E+00 2.140E+65 -14.330 128592.0 / PLOG / 1.00E+01 4.960E+61 -13.210 127269.0
/ PLOG / 2.00E+01 2.300E+57 -11.910 125334.0 / PLOG / 5.00E+01 5.700E+50 -9.950 121933.0
/ IC5H12=BC5H11+H 6.340E+18 -0.784 96250.0 PLOG / 1.00E-02 1.240E+77 -18.650 120361.0 /
PLOG / 1.00E-01 1.430E+78 -18.530 125424.0 / PLOG / 1.00E+00 2.480E+73 -16.810 126657.0 /
PLOG / 2.00E+00 3.390E+70 -15.900 125951.0 / PLOG / 5.00E+00 4.900E+65 -14.410 124153.0
/ PLOG / 1.00E+01 1.950E+61 -13.090 122150.0 / PLOG / 2.00E+01 2.310E+56 -11.630 119644.0
/ PLOG / 5.00E+01 2.030E+49 -9.560 115729.0 / IC5H12=CC5H11+H 1.740E+18 -0.685 97930.0
PLOG / 1.00E-02 7.610E+73 -17.850 119817.0 / PLOG / 1.00E-01 1.220E+76 -18.050 125581.0 /
PLOG / 1.00E+00 3.070E+72 -16.650 127663.0 / PLOG / 2.00E+00 8.790E+69 -15.820 127218.0
/ PLOG / 5.00E+00 3.060E+65 -14.440 125747.0 / PLOG / 1.00E+01 2.110E+61 -13.180 123961.0
/ PLOG / 2.00E+01 3.770E+56 -11.760 121634.0 / PLOG / 5.00E+01 4.400E+49 -9.730 117871.0
/ IC5H12=DC5H11+H 5.060E+17 -0.633 101180.0 PLOG / 1.00E-02 7.960E+67 -16.350 118712.0
/ PLOG / 1.00E-01 1.480E+72 -17.130 125626.0 / PLOG / 1.00E+00 7.210E+70 -16.360 129319.0
/ PLOG / 2.00E+00 9.510E+68 -15.710 129394.0 / PLOG / 5.00E+00 2.130E+65 -14.550 128592.0
/ PLOG / 1.00E+01 4.940E+61 -13.430 127269.0 / PLOG / 2.00E+01 2.290E+57 -12.120 125334.0
/ PLOG / 5.00E+01 5.660E+50 -10.170 121933.0 / IC5H12+O2=AC5H11+HO2 4.200E+13 0.000
52800.0 IC5H12+O2=DC5H11+HO2 2.100E+13 0.000 52800.0 IC5H12+O=AC5H11+OH 1.130E+14
0.000 7850.0 IC5H12+O=DC5H11+OH 1.050E+06 2.424 4766.0 IC5H12+H=AC5H11+H2 3.490E+05
2.690 6450.0 IC5H12+H=DC5H11+H2 1.740E+05 2.690 6450.0 IC5H12+OH=AC5H11+H2O 3.350E+06
2.078 376.0 IC5H12+OH=DC5H11+H2O 1.370E+07 1.813 868.0 IC5H12+HO2=AC5H11+H2O2
4.080E+01 3.590 17160.0 IC5H12+HO2=DC5H11+H2O2 2.040E+01 3.590 17160.0 IC5H12+CH3=AC5H11+CH4
9.040E-01 3.650 7154.0 IC5H12+CH3=DC5H11+CH4 4.520E-01 3.650 7154.0 IC5H12+CH3O=AC5H11+CH3OH
3.000E+11 0.000 7000.0 IC5H12+CH3O=DC5H11+CH3OH 1.500E+11 0.000 7000.0 IC5H12+CH3O2=AC5H11+
1.390E+00 3.970 18280.0 IC5H12+CH3O2=DC5H11+CH3O2H 6.930E-01 3.970 18280.0 IC5H12+C2H5=AC5H11
1.000E+11 0.000 13400.0 IC5H12+C2H5=DC5H11+C2H6 5.000E+10 0.000 13400.0 IC5H12+C2H3=AC5H11+C2
1.000E+12 0.000 18000.0 IC5H12+C2H3=DC5H11+C2H4 5.000E+11 0.000 18000.0 IC5H12+O2CHO=AC5H11+
1.680E+13 0.000 20440.0 IC5H12+O2CHO=DC5H11+HO2CHO 8.400E+12 0.000 20440.0 IC5H12+AC5H11=DC5
7.500E+10 0.000 12300.0 IC5H12+BC5H11=DC5H11+IC5H12 7.500E+10 0.000 12300.0 IC5H12+CC5H11=DC5H
7.500E+10 0.000 12300.0 IC5H12+O2=CC5H11+HO2 1.400E+13 0.000 50160.0 IC5H12+O=CC5H11+OH
5.950E+05 2.439 2846.0 IC5H12+H=CC5H11+H2 1.300E+06 2.400 4471.0 IC5H12+OH=CC5H11+H2O
7.050E+09 0.935 505.0 IC5H12+HO2=CC5H11+H2O2 6.320E+01 3.370 13720.0 IC5H12+CH3=CC5H11+CH4
8.400E+04 2.133 7574.0 IC5H12+CH3O=CC5H11+CH3OH 1.100E+11 0.000 5000.0 IC5H12+CH3O2=CC5H11+
1.020E+01 3.580 14810.0 IC5H12+C2H5=CC5H11+C2H6 5.000E+10 0.000 10400.0 IC5H12+C2H3=CC5H11+C2
4.000E+11 0.000 16800.0 IC5H12+O2CHO=CC5H11+HO2CHO 5.600E+12 0.000 17690.0 IC5H12+AC5H11=CC5
5.000E+10 0.000 10400.0 IC5H12+BC5H11=CC5H11+IC5H12 5.000E+10 0.000 10400.0 IC5H12+O2=BC5H11+H
7.000E+12 0.000 48000.0 IC5H12+O=BC5H11+OH 3.970E+05 2.401 1150.0 IC5H12+H=BC5H11+H2

6.020E+05 2.400 2583.0 IC5H12+OH=BC5H11+H2O 4.840E+06 1.840 -1000.0 IC5H12+HO2=BC5H11+H2O2
6.500E+02 3.010 12090.0 IC5H12+CH3=BC5H11+CH4 6.010E-10 6.360 893.0 IC5H12+CH3O=BC5H11+CH3OH
1.900E+10 0.000 2800.0 IC5H12+CH3O2=BC5H11+CH3O2H 2.620E+02 3.120 11100.0 IC5H12+C2H5=BC5H11-
1.000E+11 0.000 7900.0 IC5H12+C2H3=BC5H11+C2H4 2.000E+11 0.000 14300.0 IC5H12+O2CHO=BC5H11+H
1.500E+04 2.500 12260.0 IC5H12+AC5H11=BC5H11+IC5H12 2.500E+10 0.000 7900.0 C3H6+C2H5=AC5H11
1.420E+03 2.670 6850.0 C4H8-1+CH3=AC5H11 1.890E+03 2.670 6850.0 AC5H10+H=AC5H11
6.250E+11 0.510 2620.0 IC4H8+CH3=BC5H11 4.400E+04 2.480 6130.0 AC5H10+H=BC5H11
1.060E+12 0.510 1230.0 BC5H10+H=BC5H11 6.250E+11 0.510 2620.0 C4H8-2+CH3=CC5H11
1.890E+03 2.670 6850.0 BC5H10+H=CC5H11 2.500E+11 0.510 2620.0 CC5H10+H=CC5H11
6.250E+11 0.510 2620.0 C2H4+IC3H7=DC5H11 8.800E+03 2.480 6130.0 CC5H10+H=DC5H11
2.500E+11 0.510 2620.0 AC5H11+O2=AC5H10+HO2 8.370E-01 3.590 11960.0 BC5H11+O2=AC5H10+HO2
5.350E-01 3.710 9322.0 BC5H11+O2=BC5H10+HO2 1.070E+00 3.710 9322.0 CC5H11+O2=BC5H10+HO2
1.070E+00 3.710 9322.0 CC5H11+O2=CC5H10+HO2 5.350E-01 3.710 9322.0 DC5H11+O2=CC5H10+HO2
8.370E-01 3.590 11960.0 AC5H11=DC5H11 3.000E+11 0.000 21100.0 AC5H11+O2=AC5H11O2
6.860E+16 -1.627 199.0 BC5H11+O2=BC5H11O2 9.760E+11 0.325 -417.0 CC5H11+O2=CC5H11O2
3.490E+14 -0.816 -536.0 DC5H11+O2=DC5H11O2 6.860E+16 -1.627 199.0 AC5H11+HO2=AC5H11O+OH
9.000E+12 0.000 -1000.0 BC5H11+HO2=BC5H11O+OH 9.000E+12 0.000 -1000.0 CC5H11+HO2=CC5H11O+OH
9.000E+12 0.000 -1000.0 DC5H11+HO2=DC5H11O+OH 9.000E+12 0.000 -1000.0 AC5H11+CH3O2=AC5H11O+
9.000E+12 0.000 -1000.0 BC5H11+CH3O2=BC5H11O+CH3O 9.000E+12 0.000 -1000.0 CC5H11+CH3O2=CC5H
9.000E+12 0.000 -1000.0 DC5H11+CH3O2=DC5H11O+CH3O 9.000E+12 0.000 -1000.0 AC5H11+AC5H11O2=AC
9.000E+12 0.000 -1000.0 AC5H11+BC5H11O2=AC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
AC5H11+CC5H11O2=AC5H11O+CC5H11O 9.000E+12 0.000 -1000.0 AC5H11+DC5H11O2=AC5H11O+DC5H11
9.000E+12 0.000 -1000.0 BC5H11+AC5H11O2=BC5H11O+AC5H11O 9.000E+12 0.000 -1000.0
BC5H11+BC5H11O2=BC5H11O+BC5H11O 9.000E+12 0.000 -1000.0 BC5H11+CC5H11O2=BC5H11O+CC5H11
9.000E+12 0.000 -1000.0 BC5H11+DC5H11O2=BC5H11O+DC5H11O 9.000E+12 0.000 -1000.0
CC5H11+AC5H11O2=CC5H11O+AC5H11O 9.000E+12 0.000 -1000.0 CC5H11+BC5H11O2=CC5H11O+BC5H11
9.000E+12 0.000 -1000.0 CC5H11+CC5H11O2=CC5H11O+CC5H11O 9.000E+12 0.000 -1000.0
CC5H11+DC5H11O2=CC5H11O+DC5H11O 9.000E+12 0.000 -1000.0 DC5H11+AC5H11O2=DC5H11O+AC5H1
9.000E+12 0.000 -1000.0 DC5H11+BC5H11O2=DC5H11O+BC5H11O 9.000E+12 0.000 -1000.0
DC5H11+CC5H11O2=DC5H11O+CC5H11O 9.000E+12 0.000 -1000.0 DC5H11+DC5H11O2=DC5H11O+DC5H1
9.000E+12 0.000 -1000.0 AC5H11O2=AC5H10OOH-A 4.910E+07 1.300 21500.0 AC5H11O2=AC5H10OOH-
B 2.310E+09 0.800 27100.0 AC5H11O2=AC5H10OOH-C 1.360E+07 1.300 18200.0 AC5H11O2=AC5H10OOH-
D 1.230E+06 1.500 20000.0 BC5H11O2=BC5H10OOH-A 3.010E+09 1.200 33500.0 BC5H11O2=BC5H10OOH-
C 6.510E+09 0.700 30100.0 BC5H11O2=BC5H10OOH-D 1.500E+08 1.100 21900.0 CC5H11O2=CC5H10OOH-
A 2.880E+07 1.400 20800.0 CC5H11O2=CC5H10OOH-B 7.450E+09 0.600 27300.0 CC5H11O2=CC5H10OOH-
D 1.460E+09 1.100 33500.0 DC5H11O2=DC5H10OOH-A 2.470E+06 1.500 20000.0 DC5H11O2=DC5H10OOH-

B 1.230E+07 1.200 15400.0 DC5H11O2=DC5H10OOH-C 4.010E+08 1.100 30100.0 AC5H11O2=AC5H10+HO2
1.260E+08 1.320 28900.0 BC5H11O2=AC5H10+HO2 2.450E+10 0.890 29500.0 BC5H11O2=BC5H10+HO2
1.120E+11 0.580 29600.0 CC5H11O2=BC5H10+HO2 3.500E+10 0.710 30100.0 CC5H11O2=CC5H10+HO2
1.480E+09 1.210 29800.0 DC5H11O2=CC5H10+HO2 1.520E+07 1.660 28400.0 AC5H11O2+HO2=AC5H11O2H+
1.750E+10 0.000 -3275.0 BC5H11O2+HO2=BC5H11O2H+O2 1.750E+10 0.000 -3275.0 CC5H11O2+HO2=CC5H
1.750E+10 0.000 -3275.0 DC5H11O2+HO2=DC5H11O2H+O2 1.750E+10 0.000 -3275.0 AC5H11O2+H2O2=AC5
2.400E+12 0.000 10000.0 BC5H11O2+H2O2=BC5H11O2H+HO2 2.400E+12 0.000 10000.0 CC5H11O2+H2O2=C
2.400E+12 0.000 10000.0 DC5H11O2+H2O2=DC5H11O2H+HO2 2.400E+12 0.000 10000.0 IC5H12+AC5H11O2=
1.210E+13 0.000 20430.0 IC5H12+BC5H11O2=AC5H11+BC5H11O2H 1.210E+13 0.000 20430.0
IC5H12+CC5H11O2=AC5H11+CC5H11O2H 1.210E+13 0.000 20430.0 IC5H12+DC5H11O2=AC5H11+DC5H11O
1.210E+13 0.000 20430.0 IC5H12+AC5H11O2=DC5H11+AC5H11O2H 6.050E+12 0.000 20430.0
IC5H12+BC5H11O2=DC5H11+BC5H11O2H 6.050E+12 0.000 20430.0 IC5H12+CC5H11O2=DC5H11+CC5H11O
6.050E+12 0.000 20430.0 IC5H12+DC5H11O2=DC5H11+DC5H11O2H 6.050E+12 0.000 20430.0
IC5H12+AC5H11O2=CC5H11+AC5H11O2H 4.030E+12 0.000 17700.0 IC5H12+BC5H11O2=CC5H11+BC5H11O
4.030E+12 0.000 17700.0 IC5H12+CC5H11O2=CC5H11+CC5H11O2H 4.030E+12 0.000 17700.0
IC5H12+DC5H11O2=CC5H11+DC5H11O2H 4.030E+12 0.000 17700.0 IC5H12+AC5H11O2=BC5H11+AC5H11O
2.020E+12 0.000 16000.0 IC5H12+BC5H11O2=BC5H11+BC5H11O2H 2.020E+12 0.000 16000.0
IC5H12+CC5H11O2=BC5H11+CC5H11O2H 2.020E+12 0.000 16000.0 IC5H12+DC5H11O2=BC5H11+DC5H11O
2.020E+12 0.000 16000.0 AC5H11O2+CH3O2=¿AC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0
BC5H11O2+CH3O2=¿BC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0 CC5H11O2+CH3O2=¿CC5H11O+CH3O-
1.400E+16 -1.610 1860.0 DC5H11O2+CH3O2=¿DC5H11O+CH3O+O2 1.400E+16 -1.610 1860.0
AC5H11O2+AC5H11O2=¿AC5H11O+AC5H11O+O2 1.400E+16 -1.610 1860.0 AC5H11O2+BC5H11O2=¿AC5H1
1.400E+16 -1.610 1860.0 AC5H11O2+CC5H11O2=¿AC5H11O+CC5H11O+O2 1.400E+16 -1.610
1860.0 AC5H11O2+DC5H11O2=¿AC5H11O+DC5H11O+O2 1.400E+16 -1.610 1860.0 BC5H11O2+BC5H11O2=¿
1.400E+16 -1.610 1860.0 BC5H11O2+CC5H11O2=¿BC5H11O+CC5H11O+O2 1.400E+16 -1.610
1860.0 BC5H11O2+DC5H11O2=¿BC5H11O+DC5H11O+O2 1.400E+16 -1.610 1860.0 CC5H11O2+CC5H11O2=¿
1.400E+16 -1.610 1860.0 CC5H11O2+DC5H11O2=¿CC5H11O+DC5H11O+O2 1.400E+16 -1.610
1860.0 DC5H11O2+DC5H11O2=¿DC5H11O+DC5H11O+O2 1.400E+16 -1.610 1860.0 AC5H11O2H=AC5H11O+
3.030E+20 -1.414 46072.0 BC5H11O2H=BC5H11O+OH 8.620E+20 -1.641 45156.0 CC5H11O2H=CC5H11O+OH
1.130E+21 -1.555 45777.0 DC5H11O2H=DC5H11O+OH 3.590E+20 -1.436 46104.0 CH2O+SC4H9=AC5H11O
5.000E+10 0.000 2330.0 C2H5+CH3COCH3=BC5H11O 8.330E+09 0.000 7240.0 CH3CHO+IC3H7=CC5H11O
1.660E+10 0.000 5230.0 CH2O+IC4H9=DC5H11O 5.000E+10 0.000 2330.0 AC5H10OOH-A=A-
AC5H10O+OH 4.100E+10 0.360 17200.0 AC5H10OOH-B=A-BC5H10O+OH 7.190E+09 0.880
9600.0 AC5H10OOH-C=A-CC5H10O+OH 1.700E+09 0.734 14983.0 AC5H10OOH-D=A-DC5H10O+OH
5.200E+08 0.670 10500.0 BC5H10OOH-A=A-BC5H10O+OH 1.050E+12 0.150 9600.0 BC5H10OOH-
C=B-CC5H10O+OH 4.270E+10 0.520 8800.0 BC5H10OOH-D=B-DC5H10O+OH 1.030E+10 0.550

16200.0 CC5H10OOH-A=A-CC5H10O+OH 3.790E+07 1.517 16033.0 CC5H10OOH-B=B-CC5H10O+OH 5.360E+10 0.540 8900.0 CC5H10OOH-D=C-DC5H10O+OH 1.530E+10 0.640 10500.0 DC5H10OOH-A=A-DC5H10O+OH 5.200E+08 0.670 10500.0 DC5H10OOH-B=B-DC5H10O+OH 2.850E+08 0.920 13400.0 DC5H10OOH-C=C-DC5H10O+OH 1.120E+10 0.820 10900.0 AC5H10OOH-B=AC5H10+HO2 8.380E+09 0.920 14500.0 BC5H10OOH-A=AC5H10+HO2 3.890E+13 -0.150 15500.0 BC5H10OOH-C=BC5H10+HO2 3.010E+11 0.350 15200.0 CC5H10OOH-B=BC5H10+HO2 9.790E+12 0.040 15400.0 CC5H10OOH-D=CC5H10+HO2 6.830E+09 0.920 15100.0 DC5H10OOH-C=CC5H10+HO2 6.240E+10 0.720 15000.0 AC5H10OOH-C=¿OH+CH2O+C4H8-2 1.960E+09 1.200 23400.0 AC5H10OOH-A=¿OH+CH2O+C4H8-1 8.280E+13 -0.170 30090.0 BC5H10OOH-D=¿OH+CH3COCH3+C2H4 1.180E+20 -2.060 24210.0 CC5H10OOH-A=¿OH+CH3CHO+C3H6 3.530E+09 1.200 21900.0 DC5H10OOH-B=¿OH+CH2O+IC4H8 6.270E+08 1.400 23600.0 AC5H10OOH-A+O2=AC5H10OOH-AO2 3.090E+16 -1.627 199.0 AC5H10OOH-B+O2=AC5H10OOH-BO2 4.390E+11 0.325 -417.0 AC5H10OOH-C+O2=AC5H10OOH-CO2 1.570E+14 -0.816 -536.0 AC5H10OOH-D+O2=AC5H10OOH-DO2 3.090E+16 -1.627 199.0 BC5H10OOH-A+O2=BC5H10OOH-AO2 3.090E+16 -1.627 199.0 BC5H10OOH-C+O2=BC5H10OOH-CO2 1.570E+14 -0.816 -536.0 BC5H10OOH-D+O2=BC5H10OOH-DO2 3.090E+16 -1.627 199.0 CC5H10OOH-A+O2=CC5H10OOH-AO2 3.090E+16 -1.627 199.0 CC5H10OOH-B+O2=CC5H10OOH-BO2 4.390E+11 0.325 -417.0 CC5H10OOH-D+O2=CC5H10OOH-DO2 3.090E+16 -1.627 199.0 DC5H10OOH-A+O2=DC5H10OOH-AO2 3.090E+16 -1.627 199.0 DC5H10OOH-B+O2=DC5H10OOH-BO2 4.390E+11 0.325 -417.0 DC5H10OOH-C+O2=DC5H10OOH-CO2 1.570E+14 -0.816 -536.0 AC5H10OOH-AO2=C5H9A-AOOH+HO2 1.260E+08 1.320 28900.0 AC5H10OOH-BO2=C5H9A-AOOH+HO2 2.450E+10 0.890 29500.0 AC5H10OOH-BO2=C5H9B-AOOH+HO2 1.120E+11 0.580 29600.0 AC5H10OOH-CO2=C5H9B-AOOH+HO2 3.500E+10 0.710 30100.0 AC5H10OOH-CO2=C5H9C-AOOH+HO2 1.480E+09 1.210 29800.0 AC5H10OOH-DO2=C5H9C-AOOH+HO2 1.520E+07 1.660 28400.0 BC5H10OOH-CO2=C5H9C-BOOH+HO2 1.480E+09 1.210 29800.0 BC5H10OOH-DO2=C5H9C-BOOH+HO2 1.520E+07 1.660 28400.0 CC5H10OOH-AO2=C5H9A-COOH+HO2 1.260E+08 1.320 28900.0 CC5H10OOH-BO2=C5H9A-COOH+HO2 2.450E+10 0.890 29500.0 DC5H10OOH-AO2=C5H9A-DOOH+HO2 1.260E+08 1.320 28900.0 DC5H10OOH-BO2=C5H9A-DOOH+HO2 2.450E+10 0.890 29500.0 DC5H10OOH-BO2=C5H9B-DOOH+HO2 1.120E+11 0.580 29600.0 DC5H10OOH-CO2=C5H9B-DOOH+HO2 3.500E+10 0.710 30100.0 AC5H10OOH-AO2=C5H9B-A,AOOH 2.310E+09 0.800 27100.0 AC5H10OOH-AO2=C5H9C-A,AOOH 1.360E+07 1.300 18200.0 AC5H10OOH-AO2=C5H9D-A,AOOH 1.230E+06 1.500 20000.0 AC5H10OOH-BO2=C5H9A-A,BOOH 3.010E+09 1.200 33500.0 AC5H10OOH-BO2=C5H9C-A,BOOH 6.510E+09 0.700 30100.0 AC5H10OOH-BO2=C5H9D-A,BOOH 1.500E+08 1.100 21900.0 AC5H10OOH-CO2=C5H9A-A,COOH 2.880E+07 1.400 20800.0 AC5H10OOH-CO2=C5H9B-A,COOH 7.450E+09 0.600 27300.0 AC5H10OOH-CO2=C5H9D-A,COOH 1.460E+09 1.100 33500.0 AC5H10OOH-DO2=C5H9A-A,DOOH 2.470E+06 1.500 20000.0 AC5H10OOH-DO2=C5H9B-A,DOOH 1.230E+07 1.200 15400.0 AC5H10OOH-DO2=C5H9C-A,DOOH 4.010E+08 1.100 30100.0

BC5H10OOH-AO2=C5H9A-A,BOOH 4.910E+07 1.300 21500.0 BC5H10OOH-AO2=C5H9C-A,BOOH 1.360E+07 1.300 18200.0 BC5H10OOH-AO2=C5H9D-A,BOOH 1.230E+06 1.500 20000.0 BC5H10OOH-CO2=C5H9A-B,COOH 2.880E+07 1.400 20800.0 BC5H10OOH-CO2=C5H9D-B,COOH 1.460E+09 1.100 33500.0 BC5H10OOH-DO2=C5H9A-B,DOOH 2.470E+06 1.500 20000.0 BC5H10OOH-DO2=C5H9C-B,DOOH 4.010E+08 1.100 30100.0 CC5H10OOH-AO2=C5H9A-A,COOH 4.910E+07 1.300 21500.0 CC5H10OOH-AO2=C5H9B-A,COOH 2.310E+09 0.800 27100.0 CC5H10OOH-AO2=C5H9D-A,COOH 1.230E+06 1.500 20000.0 CC5H10OOH-BO2=C5H9A-B,COOH 3.010E+09 1.200 33500.0 CC5H10OOH-BO2=C5H9D-B,COOH 1.500E+08 1.100 21900.0 CC5H10OOH-DO2=C5H9A-C,DOOH 2.470E+06 1.500 20000.0 CC5H10OOH-DO2=C5H9B-C,DOOH 1.230E+07 1.200 15400.0 DC5H10OOH-AO2=C5H9A-A,DOOH 4.910E+07 1.300 21500.0 DC5H10OOH-AO2=C5H9B-A,DOOH 2.310E+09 0.800 27100.0 DC5H10OOH-AO2=C5H9C-A,DOOH 1.360E+07 1.300 18200.0 DC5H10OOH-BO2=C5H9A-B,DOOH 3.010E+09 1.200 33500.0 DC5H10OOH-BO2=C5H9C-B,DOOH 6.510E+09 0.700 30100.0 DC5H10OOH-CO2=C5H9A-C,DOOH 2.880E+07 1.400 20800.0 DC5H10OOH-CO2=C5H9B-C,DOOH 7.450E+09 0.600 27300.0 AC5H10OOH-AO2=IC5KETAA+OH 5.190E+04 1.900 18800.0 AC5H10OOH-BO2=IC5KETAB+OH 2.440E+07 1.600 27900.0 AC5H10OOH-CO2=IC5KETAC+OH 1.100E+04 2.400 19900.0 AC5H10OOH-DO2=IC5KETAD+OH 4.770E+03 1.700 16600.0 CC5H10OOH-AO2=IC5KETCA+OH 5.790E+01 2.900 17000.0 CC5H10OOH-BO2=IC5KETCB+OH 1.750E+08 1.700 26000.0 CC5H10OOH-DO2=IC5KETCD+OH 2.760E+08 1.200 25700.0 DC5H10OOH-AO2=IC5KETDA+OH 4.770E+03 1.700 16600.0 DC5H10OOH-BO2=IC5KETDB+OH 1.100E+04 2.400 19900.0 DC5H10OOH-CO2=IC5KETDC+OH 2.440E+07 1.600 27900.0 C5H9A-A,COOH=¿AC4H7OOH+CH2O+OH 1.980E+08 1.521 21890.0 C5H9A-A,DOOH=AC3H5O 1.980E+08 1.521 21890.0 C5H9A-C,DOOH=¿C3H6+HO2CH2CHO+OH 3.530E+09 1.200 21900.0 C5H9C-A,AOOH=¿C4H72-1OOH+CH2O+OH 1.960E+09 1.200 23400.0 C5H9D-A,AOOH=¿AC3H5OOH+C2H4+ 1.980E+08 1.521 21890.0 C5H9D-A,BOOH=¿IC3H5Q+C2H4+HO2 1.960E+09 1.200 23400.0 IC5KETAA=IC5KET 1.500E+16 0.000 42000.0 IC5KETAB=IC5KETABO+OH 6.000E+15 0.000 41200.0 IC5KETAC=IC5KETACO+OH 1.050E+16 0.000 41600.0 IC5KETAD=IC5KETADO+OH 1.500E+16 0.000 42000.0 IC5KETCA=IC5KETCAO+OH 1.500E+16 0.000 42000.0 IC5KETCB=IC5KETCBO+OH 6.000E+15 0.000 41200.0 IC5KETCD=IC5KETCDO+OH 1.500E+16 0.000 42000.0 IC5KETDA=IC5KETDAO+OH 1.500E+16 0.000 42000.0 IC5KETDB=IC5KETDBO+OH 6.000E+15 0.000 41200.0 IC5KETDC=IC5KETDCO+OH 1.050E+16 0.000 41600.0 IC5KETAAO=CH2O+C3H6CH 3 2.900E+12 0.380 11080.0 IC5KETABO=C2H5COCH3+HCO 2.900E+12 0.380 11080.0 IC5KETACO=CH3CHO+ 2.900E+12 0.380 11080.0 IC5KETADO=CH2O+IC3H6CHO 2.900E+12 0.380 11080.0 IC5KETCAO=CH2O+CH3C 2.900E+12 0.380 11080.0 IC5KETCBO=CH3COCH3+CH3CO 2.900E+12 0.380 11080.0 IC5KETCDO=CH2O+IC3 2.900E+12 0.380 11080.0 IC5KETDAO=CH2O+C3H6CHO-2 2.900E+12 0.380 11080.0 IC5KETDBO=CH3COCH3 2.900E+12 0.380 11080.0 IC5KETDCO=IC3H7CHO+HCO 2.900E+12 0.380 11080.0 C5H9A-A,BOOH=C5H9A-AOOH+HO2 3.890E+13 -0.150 15500.0 C5H9A-B,COOH=C5H9A-COOH+HO2 3.890E+13 -0.150 15500.0 C5H9A-B,DOOH=C5H9A-DOOH+HO2 3.890E+13 -0.150 15500.0 C5H9B-A,AOOH=C5H9A-AOOH+HO2 1.680E+10 0.920 14500.0 C5H9B-A,COOH=C5H9A-COOH+HO2 8.380E+09 0.920

14500.0 C5H9B-A,COOH=C5H9B-AOOH+HO2 9.790E+12 0.040 15400.0 C5H9B-A,DOOH=C5H9A-DOOH+HO2 8.380E+09 0.920 14500.0 C5H9B-C,DOOH=C5H9B-DOOH+HO2 9.790E+12 0.040 15400.0 C5H9C-A,BOOH=C5H9B-AOOH+HO2 3.010E+11 0.350 15200.0 C5H9C-A,DOOH=C5H9C-AOOH+HO2 6.240E+10 0.720 15000.0 C5H9C-B,DOOH=C5H9B-DOOH+HO2 3.010E+11 0.350 15200.0 C5H9C-B,DOOH=C5H9C-BOOH+HO2 6.240E+10 0.720 15000.0 C5H9D-A,COOH=C5H9C-AOOH+HO2 6.830E+09 0.920 15100.0 C5H9D-B,COOH=C5H9C-BOOH+HO2 6.830E+09 0.920 15100.0 C5H9A-AOOH=¿CH2O+C4H71-2+OH 1.500E+16 0.000 43000.0 C5H9A-COOH=¿CH3CHO+C3H5-T+OH 1.050E+16 0.000 42600.0 C5H9A-DOOH=¿CH2O+IC4H7+OH 1.500E+16 0.000 43000.0 C5H9B-AOOH=¿CH2O+C4H72-2+OH 1.500E+16 0.000 43000.0 C5H9B-DOOH=¿CH2O+IC4H7+OH 1.500E+16 0.000 43000.0 C5H9C-AOOH=¿CH2O+C4H71-3+OH 1.500E+16 0.000 43000.0 C5H9C-BOOH=¿CH3COCH3+C2H3+OH 6.000E+15 0.000 42200.0 C5H9A-A,BOOH=C5H9OA-AOOH-B+OH 4.100E+10 0.360 17200.0 C5H9A-A,BOOH=C5H9OA-BOOH-A+OH 1.050E+12 0.150 9600.0 C5H9A-A,COOH=C5H9OA-AOOH-C+OH 4.100E+10 0.360 17200.0 C5H9A-A,COOH=C5H9OA-COOH-A+OH 3.790E+07 1.517 16033.0 C5H9A-A,DOOH=C5H9OA-AOOH-D+OH 4.100E+10 0.360 17200.0 C5H9A-A,DOOH=C5H9OA-DOOH-A+OH 5.200E+08 0.670 10500.0 C5H9A-B,COOH=C5H9OA-BOOH-C+OH 1.050E+12 0.150 9600.0 C5H9A-B,COOH=C5H9OA-COOH-B+OH 3.790E+07 1.517 16033.0 C5H9A-B,DOOH=C5H9OA-BOOH-D+OH 1.050E+12 0.150 9600.0 C5H9A-B,DOOH=C5H9OA-DOOH-B+OH 5.200E+08 0.670 10500.0 C5H9A-C,DOOH=C5H9OA-COOH-D+OH 3.790E+07 1.517 16033.0 C5H9A-C,DOOH=C5H9OA-DOOH-C+OH 5.200E+08 0.670 10500.0 C5H9B-A,AOOH=C5H9OA-BOOH-A+OH 7.190E+09 0.880 9600.0 C5H9B-A,COOH=C5H9OA-BOOH-C+OH 7.190E+09 0.880 9600.0 C5H9B-A,COOH=C5H9OB-COOH-A+OH 5.360E+10 0.540 8900.0 C5H9B-A,DOOH=C5H9OA-BOOH-D+OH 7.190E+09 0.880 9600.0 C5H9B-A,DOOH=C5H9OB-DOOH-A+OH 2.850E+08 0.920 13400.0 C5H9B-C,DOOH=C5H9OB-COOH-D+OH 5.360E+10 0.540 8900.0 C5H9B-C,DOOH=C5H9OB-DOOH-C+OH 2.850E+08 0.920 13400.0 C5H9C-A,AOOH=C5H9OA-COOH-A+OH 1.700E+09 0.734 14983.0 C5H9C-A,BOOH=C5H9OA-COOH-B+OH 1.700E+09 0.734 14983.0 C5H9C-A,BOOH=C5H9OB-COOH-A+OH 4.270E+10 0.520 8800.0 C5H9C-A,DOOH=C5H9OA-COOH-D+OH 1.700E+09 0.734 14983.0 C5H9C-A,DOOH=C5H9OC-DOOH-A+OH 1.120E+10 0.820 10900.0 C5H9C-B,DOOH=C5H9OB-COOH-D+OH 4.270E+10 0.520 8800.0 C5H9C-B,DOOH=C5H9OC-DOOH-B+OH 1.120E+10 0.820 10900.0 C5H9D-A,AOOH=C5H9OA-DOOH-A+OH 5.200E+08 0.670 10500.0 C5H9D-A,BOOH=C5H9OA-DOOH-B+OH 5.200E+08 0.670 10500.0 C5H9D-A,BOOH=C5H9OB-DOOH-A+OH 1.030E+10 0.550 16200.0 C5H9D-A,COOH=C5H9OA-DOOH-C+OH 5.200E+08 0.670 10500.0 C5H9D-A,COOH=C5H9OC-DOOH-A+OH 1.530E+10 0.640 10500.0 C5H9D-B,COOH=C5H9OB-DOOH-C+OH 1.030E+10 0.550 16200.0 C5H9D-B,COOH=C5H9OC-DOOH-B+OH 1.530E+10 0.640 10500.0 C5H9OA-AOOH-B=¿CH2O+C2H5COCH2+OH 6.000E+15 0.000 42200.0 C5H9OA-BOOH-A=¿CH2O+C2H5COCH2+OH 1.500E+16 0.000 43000.0 C5H9OA-AOOH-C=¿CH3CHO+C3H5O+OH 1.050E+16 0.000 42600.0 C5H9OA-COOH-A=¿CH2O+C4H71-O+OH 1.500E+16 0.000 43000.0 C5H9OA-AOOH-D=¿CH2O+AC3H5OCH2-

1.500E+16 0.000 43000.0 C5H9OA-DOOH-A=¿CH2O+C4H7O1-4+OH 1.500E+16 0.000 43000.0
C5H9OA-BOOH-C=¿CH3CHO+CH3COCH2+OH 1.050E+16 0.000 42600.0 C5H9OA-COOH-B=¿CH3CHO+CH3C
6.000E+15 0.000 42200.0 C5H9OA-BOOH-D=¿CH2O+IC4H7O+OH 1.500E+16 0.000 43000.0
C5H9OA-DOOH-B=CH3COCH2OCH2CH2+OH 6.000E+15 0.000 42200.0 C5H9OA-COOH-D=¿CH2O+IC3H6CH
1.500E+16 0.000 43000.0 C5H9OA-DOOH-C=¿CH2O+IC3H6CHO+OH 1.050E+16 0.000 42600.0
C5H9OB-COOH-A=¿CH2O+CH3CHCOCH3+OH 1.500E+16 0.000 43000.0 C5H9OB-DOOH-A=¿CH2O+CH2CH
1.500E+16 0.000 43000.0 C5H9OB-COOH-D=¿CH2O+TC3H6CHO+OH 1.500E+16 0.000 43000.0
C5H9OB-DOOH-C=¿CH3COCH3+CH2CHO+OH 1.050E+16 0.000 42600.0 C5H9OC-DOOH-A=¿CH2O+C4H7O2
1+OH 1.500E+16 0.000 43000.0 C5H9OC-DOOH-B=¿CH3COCH3+CH2CHO+OH 6.000E+15 0.000
42200.0 CH3COCH2OCH2CH2=¿CH2O+C2H4+CH3CO 1.600E+13 0.000 25500.0 A-AC5H10O+OH=¿CH2O+C4
2+H2O 2.500E+12 0.000 0.0 A-BC5H10O+OH=¿IC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0 A-
CC5H10O+OH=¿C3H6+CH3CO+H2O 2.500E+12 0.000 0.0 A-DC5H10O+OH=¿C3H6+CH2CHO+H2O
2.500E+12 0.000 0.0 B-CC5H10O+OH=¿IC3H5COCH3+H+H2O 2.500E+12 0.000 0.0 B-DC5H10O+OH=¿IC4H8
2.500E+12 0.000 0.0 C-DC5H10O+OH=¿CH2CO+IC3H7+H2O 2.500E+12 0.000 0.0 A-AC5H10O+OH=¿C2H3CH
2.500E+12 0.000 0.0 A-BC5H10O+OH=¿CH2O+C4H72-2+H2O 2.500E+12 0.000 0.0 A-CC5H10O+OH=¿C3H5-
T+CH3CHO+H2O 2.500E+12 0.000 0.0 A-DC5H10O+OH=¿CH3CHCHO+C2H4+H2O 2.500E+12
0.000 0.0 B-CC5H10O+OH=¿IC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0 B-DC5H10O+OH=¿CH3COCH3+C2H
2.500E+12 0.000 0.0 C-DC5H10O+OH=¿SC3H5CHO+CH3+H2O 2.500E+12 0.000 0.0 A-AC5H10O+HO2=¿CH2
2+H2O2 5.000E+12 0.000 17700.0 A-BC5H10O+HO2=¿IC3H5CHO+CH3+H2O2 5.000E+12 0.000
17700.0 A-CC5H10O+HO2=¿C3H6+CH3CO+H2O2 5.000E+12 0.000 17700.0 A-DC5H10O+HO2=¿C3H6+CH2C
5.000E+12 0.000 17700.0 B-CC5H10O+HO2=¿IC3H5COCH3+H+H2O2 5.000E+12 0.000 17700.0
B-DC5H10O+HO2=¿IC4H8+HCO+H2O2 5.000E+12 0.000 17700.0 C-DC5H10O+HO2=¿CH2CO+IC3H7+H2O2
5.000E+12 0.000 17700.0 A-AC5H10O+HO2=¿C2H3CHO+C2H5+H2O2 5.000E+12 0.000 17700.0
A-BC5H10O+HO2=¿CH2O+C4H72-2+H2O2 5.000E+12 0.000 17700.0 A-CC5H10O+HO2=¿C3H5-
T+CH3CHO+H2O2 5.000E+12 0.000 17700.0 A-DC5H10O+HO2=¿CH3CHCHO+C2H4+H2O2
5.000E+12 0.000 17700.0 B-CC5H10O+HO2=¿IC3H5CHO+CH3+H2O2 5.000E+12 0.000 17700.0
B-DC5H10O+HO2=¿CH3COCH3+C2H3+H2O2 5.000E+12 0.000 17700.0 C-DC5H10O+HO2=¿SC3H5CHO+CH
5.000E+12 0.000 17700.0 IC3H5COCH3=IC3H5CO+CH3 1.900E+22 -1.752 83626.0 IC3H5COCH3=C3H5-
T+CH3CO 6.070E+24 -2.210 96960.0 IC3H5COCH3+OH=IC3H5COCH2+H2O 5.100E+11 0.000
1192.0 IC3H5COCH3+O=IC3H5COCH2+OH 5.000E+12 0.000 5962.0 IC3H5COCH3+H=IC3H5COCH2+H2
9.300E+12 0.000 6357.0 IC3H5COCH3+CH3=IC3H5COCH2+CH4 1.620E+11 0.000 9630.0 IC3H5COCH3+HO2=
8.500E+12 0.000 20460.0 IC3H5COCH3+O2=IC3H5COCH2+HO2 6.000E+13 0.000 46000.0 IC3H5COCH2=C3H5
T+CH2CO 5.970E+14 0.188 51272.0 IC3H5COCH3+OH=AC3H4COCH3+H2O 3.120E+06 2.000 -
298.0 IC3H5COCH3+O=AC3H4COCH3+OH 6.030E+10 0.700 7633.0 IC3H5COCH3+H=AC3H4COCH3+H2
1.730E+05 2.500 2492.0 IC3H5COCH3+CH3=AC3H4COCH3+CH4 2.210E+00 3.500 5675.0 IC3H5COCH3+HO2=
9.640E+03 2.600 13910.0 IC3H5COCH3+O2=AC3H4COCH3+HO2 6.030E+13 0.000 47590.0 AC3H4COCH3=C3H

A+CH3CO 1.400E+13 0.000 60000.0 NEOC5H12=TC4H9+CH3 1.000E+00 1.000 1.0 PLOG /
1.00E-02 2.570E+105 -26.530 123826.0 / PLOG / 1.00E-01 1.600E+101 -24.970 124575.0 / PLOG
/ 3.00E-01 8.940E+97 -23.870 124190.0 / PLOG / 1.00E+00 2.360E+93 -22.400 123102.0 / PLOG
/ 2.00E+00 1.790E+90 -21.410 122140.0 / PLOG / 5.00E+00 4.000E+85 -19.970 120475.0 /
PLOG / 1.00E+01 4.990E+81 -18.770 118913.0 / PLOG / 2.00E+01 3.100E+77 -17.490 117095.0
/ PLOG / 5.00E+01 3.550E+71 -15.710 114337.0 / PLOG / 1.00E+02 7.570E+66 -14.320 112041.0
/ NEOC5H12=NEOC5H11+H 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.020E+82 -20.610 123687.0
/ PLOG / 1.00E-01 8.020E+83 -20.760 127660.0 / PLOG / 3.00E-01 2.930E+83 -20.440 128998.0 /
PLOG / 1.00E+00 7.740E+81 -19.790 129931.0 / PLOG / 2.00E+00 2.900E+80 -19.260 130191.0 /
PLOG / 5.00E+00 9.040E+77 -18.400 130162.0 / PLOG / 1.00E+01 3.440E+75 -17.600 129792.0 /
PLOG / 2.00E+01 4.170E+72 -16.670 129063.0 / PLOG / 5.00E+01 9.620E+67 -15.220 127494.0 /
PLOG / 1.00E+02 8.760E+63 -13.990 125858.0 / NEOC5H12+O2=NEOC5H11+HO2 8.400E+13
0.000 52800.0 NEOC5H12+O=NEOC5H11+OH 2.260E+14 0.000 7850.0 NEOC5H12+H=NEOC5H11+H2
6.980E+05 2.690 6450.0 NEOC5H12+OH=NEOC5H11+H2O 6.570E+07 1.763 743.0 NEOC5H12+HO2=NEOC5H
8.160E+01 3.590 17160.0 NEOC5H12+CH3=NEOC5H11+CH4 1.810E+00 3.650 7154.0 NEOC5H12+CH3O=NEO
6.000E+11 0.000 7000.0 NEOC5H12+CH3O2=NEOC5H11+CH3O2H 2.770E+00 3.970 18280.0
NEOC5H12+C2H5=NEOC5H11+C2H6 2.000E+11 0.000 13400.0 NEOC5H12+C2H3=NEOC5H11+C2H4
2.000E+12 0.000 18000.0 NEOC5H12+O2CHO=NEOC5H11+HO2CHO 2.770E+00 3.970 18280.0
NEOC5H12+IC4H6OH=NEOC5H11+IC4H7OH 9.400E+02 3.300 19840.0 NEOC5H12+IC4H7O=NEOC5H11+IC4
5.400E+11 0.000 4000.0 NEOC5H12+TC3H6CHO=NEOC5H11+IC3H7CHO 9.400E+02 3.300 19840.0
NEOC5H12+CH2CCH2OH=NEOC5H11+C3H5OH 1.590E+12 0.000 20500.0 NEOC5H11=IC4H8+CH3
3.650E+18 -1.337 33462.0 PLOG / 1.00E-02 2.750E+32 -6.660 31143.0 / PLOG / 1.00E-01
2.650E+37 -7.680 36912.0 / PLOG / 1.00E+00 6.530E+39 -7.980 41554.0 / PLOG / 2.00E+00
1.050E+40 -7.940 42640.0 / PLOG / 5.00E+00 1.190E+40 -7.830 43859.0 / PLOG / 1.00E+01
1.130E+40 -7.750 44627.0 / PLOG / 2.00E+01 1.150E+40 -7.690 45269.0 / PLOG / 5.00E+01
1.440E+40 -7.660 45920.0 / PLOG / 1.00E+02 1.810E+40 -7.670 46255.0 / NEOC5H11+O2=NEOC5H11O2
6.860E+16 -1.627 199.0 NEOC5H11+HO2=NEOC5H11O+OH 9.000E+12 0.000 -1000.0 NEOC5H11+CH3O2=NE
9.000E+12 0.000 -1000.0 NEOC5H11+NEOC5H11O2=NEOC5H11O+NEOC5H11O 9.000E+12 0.000
-1000.0 NEOC5H11O2=NEOC5H10OOH 1.200E+09 1.200 21600.0 NEOC5H11O2+HO2=NEOC5H11O2H+O2
1.750E+10 0.000 -3275.0 NEOC5H11O2+H2O2=NEOC5H11O2H+HO2 2.400E+12 0.000 10000.0
NEOC5H12+NEOC5H11O2=NEOC5H11+NEOC5H11O2H 2.420E+13 0.000 20430.0 NEOC5H11O2+CH3O2=¿N
1.400E+16 -1.610 1860.0 NEOC5H11O2+NEOC5H11O2=¿NEOC5H11O+NEOC5H11O+O2 1.400E+16
-1.610 1860.0 NEOC5H11O2H=NEOC5H11O+OH 2.090E+17 -0.400 45110.0 CH2O+TC4H9=NEOC5H11O
5.000E+10 0.000 2330.0 NEOC5H10OOH=NEO-C5H10O+OH 3.710E+09 0.700 15900.0 NEOC5H10OOH=¿OH+
3.640E+09 1.300 23700.0 NEOC5H10OOH=IC4H7OOH+CH3 1.640E+07 2.000 28300.0 NEOC5H10OOH+O2=NE
O2 3.430E+16 -1.627 199.0 NEOC5H10OOH-O2=NEOC5H9Q2 7.990E+08 1.200 21600.0 NEOC5H10OOH-

O2=NEOC5KET+OH 5.190E+04 1.900 18800.0 NEOC5H9Q2=IC4H7OOH+CH2O2H 3.640E+09
1.300 23700.0 NEOC5H9Q2=IC4H6Q2-II+CH3 1.640E+07 2.000 28300.0 NEOC5KET=NEOC5KETOX+OH
1.500E+16 0.000 43000.0 NEOC5KETOX=TC3H6CHO+CH2O 2.480E+21 -2.540 15830.0 NEOC5H9Q2=NEOC5H
OOH+OH 3.710E+09 0.700 15900.0 NEOC5H9O-OOH=¿C3H5-T+CH2O+CH2O+OH 1.000E+16
0.000 43000.0 NEO-C5H10O+OH=TC4H8CHO+H2O 2.500E+12 0.000 0.0 NEO-C5H10O+OH=¿IC4H7+CH2O+
2.500E+12 0.000 0.0 NEO-C5H10O+HO2=TC4H8CHO+H2O2 5.000E+12 0.000 17700.0 NEO-
C5H10O+HO2=¿IC4H7+CH2O+H2O2 5.000E+12 0.000 17700.0 NEO-C5H10O+H=TC4H8CHO+H2
3.540E+07 2.000 5000.0 NEO-C5H10O+H=¿IC4H7+CH2O+H2 1.330E+06 2.540 6756.0 NEO-
C5H10O=IC4H8+CH2O 3.800E+15 0.000 60700.0 NEOC5KETOX=NEOC5KEJOL 1.200E+09 1.199
13601.0 NEOC5KEJOL=IC4H8OH+CO 2.270E+21 -2.340 11020.0 C5H10-1=C2H5+C3H5-A 1.460E+27
-3.030 78550.0 C4H71-3+CH3(+M)=C5H10-2(+M) 1.000E+14 -0.320 -262.0 LOW / 3.910E+60
-12.810 6250.0 / TROE / 1.040E-01 1.606E+03 6.000E+04 6.118E+03 / H2/ 2.00/ H2O/ 6.00/
CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ C5H10-1+O2=C5H91-5+HO2 3.000E+13
0.000 52290.0 C5H10-1+O=C5H91-5+OH 9.800E+05 2.430 4750.0 C5H10-1+H=C5H91-5+H2
6.650E+05 2.540 6756.0 C5H10-1+OH=C5H91-5+H2O 5.270E+09 0.970 1586.0 C5H10-1+HO2=C5H91-
5+H2O2 2.380E+04 2.550 16490.0 C5H10-1+CH3=C5H91-5+CH4 4.520E-01 3.650 7154.0 C5H10-
1+CH3O=C5H91-5+CH3OH 2.170E+11 0.000 6458.0 C5H10-1+CH3O2=C5H91-5+CH3O2H 2.380E+04
2.550 16490.0 C5H10-2+O2=C5H92-5+HO2 3.000E+13 0.000 52290.0 C5H10-2+O=C5H92-5+OH
9.800E+05 2.430 4750.0 C5H10-2+H=C5H92-5+H2 6.650E+05 2.540 6756.0 C5H10-2+OH=C5H92-
5+H2O 5.270E+09 0.970 1586.0 C5H10-2+HO2=C5H92-5+H2O2 2.380E+04 2.550 16490.0 C5H10-
2+CH3=C5H92-5+CH4 4.520E-01 3.650 7154.0 C5H10-2+CH3O=C5H92-5+CH3OH 2.170E+11
0.000 6458.0 C5H10-2+CH3O2=C5H92-5+CH3O2H 2.380E+04 2.550 16490.0 C5H10-1+O2=C5H91-
4+HO2 2.000E+13 0.000 49640.0 C5H10-1+O=C5H91-4+OH 5.510E+05 2.450 2830.0 C5H10-
1+H=C5H91-4+H2 1.300E+06 2.400 4471.0 C5H10-1+OH=C5H91-4+H2O 4.670E+07 1.610 -
35.0 C5H10-1+HO2=C5H91-4+H2O2 9.640E+03 2.600 13910.0 C5H10-1+CH3=C5H91-4+CH4
1.510E+00 3.460 5481.0 C5H10-1+CH3O=C5H91-4+CH3OH 1.450E+11 0.000 4571.0 C5H10-
1+CH3O2=C5H91-4+CH3O2H 9.640E+03 2.600 13910.0 C5H10-2+O2=C5H91-3+HO2 3.300E+12
0.000 39900.0 C5H10-2+O=C5H91-3+OH 4.410E+05 2.420 3150.0 C5H10-2+H=C5H91-3+H2
1.730E+05 2.500 2492.0 C5H10-2+OH=C5H91-3+H2O 3.120E+06 2.000 -298.0 C5H10-2+HO2=C5H91-
3+H2O2 9.640E+03 2.600 13910.0 C5H10-2+CH3=C5H91-3+CH4 2.210E+00 3.500 5675.0 C5H10-
2+CH3O=C5H91-3+CH3OH 9.000E+01 2.950 11990.0 C5H10-2+CH3O2=C5H91-3+CH3O2H 9.640E+03
2.600 13910.0 C5H10-1+O2=C5H91-3+HO2 2.200E+12 0.000 37220.0 C5H10-1+O=C5H91-3+OH
6.600E+05 2.430 1210.0 C5H10-1+H=C5H91-3+H2 3.380E+05 2.360 207.0 C5H10-1+OH=C5H91-
3+H2O 2.760E+04 2.640 -1919.0 C5H10-1+HO2=C5H91-3+H2O2 4.820E+03 2.550 10530.0 C5H10-
1+CH3=C5H91-3+CH4 3.690E+00 3.310 4002.0 C5H10-1+CH3O=C5H91-3+CH3OH 4.000E+01
2.900 8609.0 C5H10-1+CH3O2=C5H91-3+CH3O2H 4.820E+03 2.550 10530.0 C5H10-2+O2=C5H92-

4+HO2 2.200E+12 0.000 37220.0 C5H10-2+O=C5H92-4+OH 9.900E+05 2.430 1210.0 C5H10-
2+H=C5H92-4+H2 3.380E+05 2.360 207.0 C5H10-2+OH=C5H92-4+H2O 2.760E+04 2.640 -
1919.0 C5H10-2+HO2=C5H92-4+H2O2 4.820E+03 2.550 10530.0 C5H10-2+CH3=C5H92-4+CH4
3.690E+00 3.310 4002.0 C5H10-2+CH3O=C5H92-4+CH3OH 4.000E+01 2.900 8609.0 C5H10-
2+CH3O2=C5H92-4+CH3O2H 4.820E+03 2.550 10530.0 C5H10-1+OH=C5H10OH12 4.750E+12
0.000 -782.0 C5H10-2+OH=C5H10OH23 4.750E+12 0.000 -782.0 C5H10OH-2O2=¿NC3H7CHO+CH2O+OH
2.500E+10 0.000 18860.0 C5H10OH23+O2=O2C5H10OH23 2.000E+12 0.000 0.0 O2C5H10OH23=¿C2H5CHO+C
2.500E+10 0.000 18860.0 C4H6+CH3=C5H91-3 1.000E+11 0.000 7800.0 C5H81-3+H=C5H91-3
2.500E+11 0.510 2620.0 C3H6+C2H3=C5H91-4 1.000E+11 0.000 7800.0 C2H4+C3H5-A=C5H91-
5 1.000E+11 0.000 7800.0 C5H81-3+H=C5H92-4 4.240E+11 0.510 1230.0 C2H4+C3H5-S=C5H92-
5 2.000E+11 0.000 7800.0 C5H9O1-3+OH=C5H91-3+HO2 6.090E+15 -1.070 15720.0 C5H9O1-
3+CH3O=C5H91-3+CH3O2 5.950E+17 -1.650 20480.0 C5H9O1-3+C2H5O=C5H91-3+C2H5O2
3.890E+14 -0.720 18330.0 C5H9O2-4+OH=C5H92-4+HO2 7.030E+15 -1.240 15890.0 C5H9O2-
4+CH3O=C5H92-4+CH3O2 6.860E+17 -1.820 20650.0 C5H9O2-4+C2H5O=C5H92-4+C2H5O2
4.490E+14 -0.890 18490.0 C5H9O1-3=C2H3CHO+C2H5 3.130E+19 -1.850 10670.0 C5H9O1-3=C2H5CHO+C2H3
1.420E+18 -1.560 23340.0 C5H9O2-4=SC3H5CHO+CH3 5.980E+15 -1.130 9941.0 C5H9O2-4=CH3CHO+C3H5-
S 1.070E+22 -2.660 29650.0 BC5H10=C4H72-2+CH3 1.220E+23 -1.926 101400.0 BC5H10=IC4H7-
I1+CH3 2.150E+64 -13.400 135000.0 DUP BC5H10=IC4H7-I1+CH3 7.290E+38 -6.700 108740.0
DUP C4H71-3+CH3(+M)=CC5H10(+M) 1.000E+14 -0.320 -262.0 LOW / 3.910E+60 -12.810
6250.0 / TROE / 1.040E-01 1.606E+03 6.000E+04 6.118E+03 / H2/ 2.00/ H2O/ 6.00/ CH4/
2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ CC5H10+H=CC5H9-A+H2 3.900E+06 2.400
4471.0 CC5H10+OH=CC5H9-A+H2O 1.400E+08 1.610 -35.0 CC5H10+HO2=CC5H9-A+H2O2
2.890E+04 2.600 13910.0 CC5H10+CH3=CC5H9-A+CH4 4.530E+00 3.460 5481.0 CC5H10+CH3O=CC5H9-
A+CH3OH 4.350E+11 0.000 4571.0 CC5H10+CH3O2=CC5H9-A+CH3O2H 2.890E+04 2.600 13910.0
BC5H10+H=AC5H9-C+H2 3.460E+05 2.500 2492.0 BC5H10+H=CC5H9-B+H2 1.730E+05 2.500
2492.0 BC5H10+OH=AC5H9-C+H2O 6.240E+06 2.000 -298.0 BC5H10+OH=CC5H9-B+H2O 3.120E+06
2.000 -298.0 BC5H10+HO2=AC5H9-C+H2O2 1.930E+04 2.600 13910.0 BC5H10+HO2=CC5H9-
B+H2O2 9.640E+03 2.600 13910.0 BC5H10+CH3=AC5H9-C+CH4 4.420E+00 3.500 5675.0 BC5H10+CH3=CC5H
B+CH4 2.210E+00 3.500 5675.0 BC5H10+CH3O=AC5H9-C+CH3OH 1.800E+02 2.950 11990.0
BC5H10+CH3O=CC5H9-B+CH3OH 9.000E+01 2.950 11990.0 BC5H10+CH3O2=AC5H9-C+CH3O2H
1.930E+04 2.600 13910.0 BC5H10+CH3O2=CC5H9-B+CH3O2H 9.640E+03 2.600 13910.0 CC5H10+H=CC5H9-
B+H2 2.650E+06 2.200 0.0 CC5H10+OH=CC5H9-B+H2O 6.140E+02 3.200 -3500.0 CC5H10+HO2=CC5H9-
B+H2O2 1.810E+03 2.500 7154.0 CC5H10+CH3=CC5H9-B+CH4 4.610E+00 3.100 2330.0 CC5H10+CH3O=CC5H
B+CH3OH 1.000E+01 2.850 5231.0 CC5H10+CH3O2=CC5H9-B+CH3O2H 1.810E+03 2.500 7154.0
BC5H10+OH=BC5H10OH 1.000E+12 0.000 -1042.0 BC5H10OH+O2=BO2C5H10OH 2.000E+12
0.000 0.0 BO2C5H10OH=¿CH3COCH3+CH3CHO+OH 2.500E+10 0.000 18860.0 CC5H10+OH=CC5H10OH

1.000E+12 0.000 -1042.0 CC5H10OH+O2=CO2C5H10OH 2.000E+12 0.000 0.0 CO2C5H10OH=¿IC3H7CHO+CH2
2.500E+10 0.000 18860.0 BC5H10+OH=IC3H7+CH3CHO 2.000E+10 0.000 4000.0 CC5H10+OH=IC4H9+CH2O
2.000E+10 0.000 4000.0 AC5H9-A2+HO2=AC5H9O-A2+OH 9.640E+12 0.000 0.0 AC5H9-A2+CH3O2=AC5H9O-
A2+CH3O 9.640E+12 0.000 0.0 AC5H9-A2+C2H5O2=AC5H9O-A2+C2H5O 9.640E+12 0.000 0.0
CC5H9-B+HO2=CC5H9O-B+OH 7.000E+12 0.000 -1000.0 CC5H9-B+CH3O2=CC5H9O-B+CH3O
7.000E+12 0.000 -1000.0 CC5H9-B+C2H5O2=CC5H9O-B+C2H5O 9.640E+12 0.000 0.0 AC5H9O-
A2=C4H71-2+CH2O 9.210E+17 -1.430 30330.0 AC5H9-D=AC5H9-A2 1.110E+12 0.000 31700.0
AC5H10=C3H5-T+C2H5 8.920E+24 -2.409 100500.0 IC4H7+CH3(+M)=AC5H10(+M) 1.500E+14
-0.320 -262.0 LOW / 5.860E+60 -12.810 6250.0 / TROE / 1.040E-01 1.606E+03 6.000E+04
6.118E+03 / H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/
AC5H10+H=AC5H9-A2+H2 1.730E+05 2.500 2492.0 AC5H10+O=AC5H9-A2+OH 3.700E+05
2.560 -1130.0 AC5H10+OH=AC5H9-A2+H2O 3.120E+06 2.000 -298.0 AC5H10+HO2=AC5H9-
A2+H2O2 9.640E+03 2.600 13910.0 AC5H10+CH3=AC5H9-A2+CH4 2.210E+00 3.500 5675.0
AC5H10+CH3O2=AC5H9-A2+CH3O2H 9.640E+03 2.600 13910.0 AC5H10+CH3O=AC5H9-A2+CH3OH
9.000E+01 2.950 11990.0

AC5H10+H=AC5H9-C+H2 3.380E+05 2.360 207.0 AC5H10+OH=AC5H9-C+H2O 2.760E+04
2.640 -1919.0 AC5H10+HO2=AC5H9-C+H2O2 4.820E+03 2.550 10530.0 AC5H10+CH3=AC5H9-
C+CH4 3.690E+00 3.310 4002.0 AC5H10+CH3O2=AC5H9-C+CH3O2H 4.820E+03 2.550 10530.0
AC5H10+CH3O=AC5H9-C+CH3OH 4.000E+01 2.900 8609.0 AC5H10+H=AC5H9-D+H2 1.950E+06
2.400 4471.0 AC5H10+OH=AC5H9-D+H2O 7.010E+07 1.610 -35.0 AC5H10+CH3=AC5H9-D+CH4
2.270E+00 3.460 5481.0 AC5H10+HO2=AC5H9-D+H2O2 1.450E+04 2.600 13910.0 AC5H10+CH3O=AC5H9-
D+CH3OH 2.180E+11 0.000 4571.0 AC5H10+CH3O2=AC5H9-D+CH3O2H 1.450E+04 2.600 13910.0
AC5H9-A2=C3H4-A+C2H5 1.980E+20 -1.630 59240.0 B13DE2M+H=AC5H9-C 4.000E+13 0.000
1300.0 C4H612+CH3=AC5H9-C 1.760E+04 2.480 6130.0 B13DE2M+H=AC5H9-D 2.500E+11
0.510 2620.0 AC5H9-D=C3H5-T+C2H4 1.220E+12 0.640 29370.0 AC5H10+OH=SC4H9+CH2O
2.000E+10 0.000 4000.0 AC5H10+OH=AC5H10OH 1.000E+12 0.000 -1042.0 AC5H10OH+O2=AO2C5H10OH
2.000E+12 0.000 0.0 AO2C5H10OH=¿C2H5COCH3+CH2O+OH 2.500E+10 0.000 18860.0 AC5H10+O=SC4H9+
7.230E+05 2.340 -1050.0 AC5H10+O=IC3H7+CH3CO 7.230E+05 2.340 -1050.0 AC5H10+O=IC4H9+HCO
7.230E+05 2.340 -1050.0 AC5H9-C+HO2=AC5H9O-C+OH 7.000E+12 0.000 -1000.0 AC5H9-
C+CH3O2=AC5H9O-C+CH3O 7.000E+12 0.000 -1000.0 AC5H9-C+C2H5O2=AC5H9O-C+C2H5O
9.640E+12 0.000 0.0 CH3CHO+C3H5-T=AC5H9O-C 9.450E+02 2.670 6850.0

AC5H9-C+HO2=B2E2M1OJ+OH 7.000E+12 0.000 -1000.0 AC5H9-C+CH3O2=B2E2M1OJ+CH3O
7.000E+12 0.000 -1000.0 CH2O+C4H72-2=B2E2M1OJ 8.800E+03 2.480 6100.0

C2H3+C3H5-T=B13DE2M 8.000E+12 0.000 0.0 H+B13DE2MJ=B13DE2M 1.000E+14 0.000

0.0 B13DE2M+H=B13DE2MJ+H2 3.640E+05 2.455 4361.0 B13DE2M+O2=B13DE2MJ+HO2
5.960E+19 -1.670 46192.0 B13DE2M+OH=B13DE2MJ+H2O 4.460E+06 2.072 1051.0 B13DE2M+HO2=B13DE2
3.070E-02 4.403 13547.0 B13DE2M+CH3=B13DE2MJ+CH4 2.210E+00 3.500 5675.0 B13DE2M+CH3O2=B13DE
7.680E-02 4.403 13547.0 C2H3+C3H4-A=B13DE2MJ 9.450E+02 2.670 6850.0 B13DE2M+H=CC5H9-
B 4.240E+11 0.510 1230.0 B13DE2M+H=CC5H9-A 2.500E+11 0.510 2620.0 B12DE3M+H=CC5H9-
B 4.240E+11 0.510 1230.0

C2H3+C3H6=CC5H9-A 9.450E+02 2.670 6850.0

C2H3+CH3COCH3=CC5H9O-B 9.450E+02 2.670 6850.0 CC5H9-B+HO2=B2E3M1OJ+OH
7.000E+12 0.000 -1000.0 CC5H9-B+CH3O2=B2E3M1OJ+CH3O 7.000E+12 0.000 -1000.0 CH2O+IC4H7-
I1=B2E3M1OJ 8.800E+03 2.480 6100.0 TC4H8CHO=IC3H5CHO+CH3 1.000E+13 0.000 26290.0
TC4H8CHO=IC4H8+HCO 8.520E+12 0.000 20090.0 TC4H8CHO+O2=O2C4H8CHO 2.000E+12
0.000 0.0 O2C4H8CHO=O2HC4H8CO 2.160E+11 0.000 15360.0 IC4H8O2H-T+CO=O2HC4H8CO
1.500E+11 0.000 4809.0 C2H5+C2H3CHO=PC4H8CHO-1 1.000E+11 0.000 7800.0 CH3+AC3H5CHO=PC4H8CH
2 1.000E+11 0.000 7800.0 C4H8-1+HCO=PC4H8CHO-2 1.000E+11 0.000 6000.0 C3H6+CH2CHO=PC4H8CHO-
3 1.000E+11 0.000 7800.0 C2H4+CH2CH2CHO=PC4H8CHO-4 1.000E+11 0.000 7800.0 C3H5-
A+HCO=AC3H5CHO 1.810E+13 0.000 0.0 PC4H9CHO+O2=PC4H9CO+HO2 3.010E+13 0.000
39150.0 PC4H9CHO+O=PC4H9CO+OH 5.940E+12 0.000 1868.0 PC4H9CHO+H=PC4H9CO+H2
1.310E+05 2.580 1220.0 PC4H9CHO+OH=PC4H9CO+H2O 3.370E+12 0.000 -619.0 PC4H9CHO+HO2=PC4H9C
3.010E+12 0.000 11920.0 PC4H9CHO+CH3=PC4H9CO+CH4 7.080E-04 4.580 1966.0 PC4H9CHO+CH3O2=PC4
3.010E+12 0.000 11920.0 PC4H9CHO+OH=PC4H8CHO-1+H2O 5.520E+02 3.120 -1176.0 PC4H9CHO+OH=PC4
2+H2O 4.680E+07 1.610 -35.0 PC4H9CHO+OH=PC4H8CHO-3+H2O 4.680E+07 1.610 -35.0
PC4H9CHO+OH=PC4H8CHO-4+H2O 5.280E+09 0.970 1586.0 PC4H9CHO+HO2=PC4H8CHO-
1+H2O2 3.440E+12 0.050 17880.0 PC4H9CHO+HO2=PC4H8CHO-2+H2O2 9.640E+03 2.600
13910.0 PC4H9CHO+HO2=PC4H8CHO-3+H2O2 9.640E+03 2.600 13910.0 PC4H9CHO+HO2=PC4H8CHO-
4+H2O2 2.380E+04 2.550 16490.0 PC4H9CHO+CH3O2=PC4H8CHO-1+CH3O2H 3.440E+12 0.050
17880.0 PC4H9CHO+CH3O2=PC4H8CHO-2+CH3O2H 9.640E+03 2.600 13910.0 PC4H9CHO+CH3O2=PC4H8C
3+CH3O2H 9.640E+03 2.600 13910.0 PC4H9CHO+CH3O2=PC4H8CHO-4+CH3O2H 2.380E+04
2.550 16490.0 NC3H7+CH2CO=PC4H9CO 3.330E+02 2.730 13954.0 PC4H9CO=PC4H9+CO 5.780E+14
0.000 16844.0 PC4H8CHO-1+O2=PC4H8CHO-1O2 1.000E+11 0.000 0.0 PC4H8CHO-2+O2=PC4H8CHO-
2O2 3.490E+14 -0.816 -536.0 PC4H8CHO-3+O2=PC4H8CHO-3O2 3.490E+14 -0.816 -536.0 PC4H8CHO-
4+O2=PC4H8CHO-4O2 6.860E+16 -1.627 199.0 PC4H8CHO-1O2=C4H7CHO-2+HO2 2.880E+09
0.930 29800.0 PC4H8CHO-2O2=C4H7CHO-2+HO2 2.880E+09 0.930 29800.0 PC4H8CHO-2O2=C4H7CHO-
3+HO2 2.880E+09 0.930 29800.0 PC4H8CHO-3O2=C4H7CHO-3+HO2 2.880E+09 0.930 29800.0
PC4H8CHO-3O2=C4H7CHO-4+HO2 2.880E+09 0.930 29800.0 PC4H8CHO-4O2=C4H7CHO-4+HO2
2.880E+09 0.930 29800.0 C4H7CHO-2+OH=¿C4H71-1+CO+H2O 1.700E+12 0.000 -619.0 C4H7CHO-

3+OH=¿C4H72-2+CO+H2O 1.700E+12 0.000 -619.0 C4H7CHO-3+OH=¿C4H6+HCO+H2O 1.010E+06
2.200 -437.0 C4H7CHO-4+OH=¿C4H71-4+CO+H2O 1.700E+12 0.000 -619.0 C4H7CHO-4+OH=¿C4H6+HCO+H
1.010E+06 2.200 -437.0 C3H5O+C2H4=C5H9O12-5 1.000E+11 0.000 12000.0 CH2CH2CHO+C2H4=C5H9O13-
5 1.000E+11 0.000 12000.0 CH2O+C4H71-4=C5H9O14-5 1.000E+11 0.000 12000.0 C2H3CHO+C2H5=C5H9O23-
1 1.000E+11 0.000 12000.0 CH3CHCHO+C2H4=C5H9O23-5 1.000E+11 0.000 12000.0 CH3CHO+C3H5-
A=C5H9O24-1 1.000E+11 0.000 12000.0 CH3CO+NC3H7=NC3H7COCH3 2.000E+13 0.000 0.0
NC3H7COCH3+OH=NC3H7COCH2+H2O 3.990E+02 3.080 944.0 NC3H7COCH3+HO2=NC3H7COCH2+H2O2
4.140E-02 4.070 16253.0 NC3H7COCH3+OH=CH3CH2CHCOCH3+H2O 2.360E+02 3.150 3050.0
NC3H7COCH3+HO2=CH3CH2CHCOCH3+H2O2 3.560E-01 3.690 13100.0 NC3H7COCH3+OH=CH3CHCH2COC
4.140E+02 3.000 2440.0 NC3H7COCH3+HO2=CH3CHCH2COCH3+H2O2 1.150E-03 4.430 11365.0
NC3H7COCH3+OH=CH2CH2CH2COCH3+H2O 2.730E+07 1.813 868.0 NC3H7COCH3+HO2=CH2CH2CH2COC
4.440E-01 3.880 15814.0 C2H5COC2H5+OH=CH2CH2COC2H5+H2O 2.700E+00 3.810 2899.0
C2H5COC2H5+HO2=CH2CH2COC2H5+H2O2 6.180E-05 4.910 14081.0 C2H5COC2H5+OH=CH3CHCOC2H5+H
2.360E+02 3.150 3050.0 C2H5COC2H5+HO2=CH3CHCOC2H5+H2O2 8.420E-02 3.930 13390.0
NC3H7+CH2CO=NC3H7COCH2 3.630E+03 2.430 8960.0 C2H3COCH3+CH3=CH3CH2CHCOCH3
1.760E+04 2.480 6130.0 C3H6+CH3CO=CH3CHCH2COCH3 8.800E+03 2.480 6130.0 C2H4+CH3COCH2=CH2CH
1.320E+04 2.480 6130.0 C2H4+C2H5CO=CH2CH2COC2H5 8.800E+03 2.480 6130.0 CH3CHCO+C2H5=CH3CHC
3.630E+03 2.430 8960.0 CH3CH2CHCOCH3+O2=NC52ONEO2-3 1.000E+11 0.000 0.0 CH3CHCH2COCH3+O2=
4 3.490E+14 -0.816 -536.0 CH2CH2CH2COCH3+O2=NC52ONEO2-5 6.860E+16 -1.627 199.0
CH2CH2COC2H5+O2=NC53ONEO2-1 6.860E+16 -1.627 199.0 CH3CHCOC2H5+O2=NC53ONEO2-
2 1.000E+11 0.000 0.0 NC52ONEO2-3=NC52ONE-3+HO2 2.880E+09 0.930 29800.0 NC52ONEO2-
4=NC52ONE-3+HO2 2.880E+09 0.930 29800.0 NC52ONEO2-4=NC52ONE-4+HO2 2.880E+09
0.930 29800.0 NC52ONEO2-5=NC52ONE-4+HO2 2.880E+09 0.930 29800.0 NC53ONEO2-1=NC53ONE-
1+HO2 2.880E+09 0.930 29800.0 NC53ONEO2-2=NC53ONE-1+HO2 2.880E+09 0.930 29800.0
NC52ONE-3+OH=¿CH2CO+C3H5-S+H2O 4.460E+06 2.072 1051.0 NC52ONE-4+OH=¿CH2CO+C3H5-
A+H2O 1.010E+06 2.200 -437.0 NC53ONE-1+OH=¿CH3CHCO+C2H3+H2O 2.360E+02 3.150
3050.0 NC5H11OH+OH=C5H10OH15+H2O 5.280E+09 0.970 1590.0 NC5H11OH+HO2=C5H10OH15+H2O2
2.040E+01 3.590 17160.0 NC5H11OH+OH=C5H10OH14+H2O 4.670E+07 1.610 -35.0 NC5H11OH+HO2=C5H10
6.320E+01 3.370 13720.0 NC5H11OH+OH=C5H10OH13+H2O 1.140E+03 2.870 -2926.0 NC5H11OH+HO2=C5H
2.760E-04 4.760 11850.0 NC5H11OH+OH=C5H10OH12+H2O 1.540E+00 3.700 -3736.0 NC5H11OH+HO2=C5H1
7.510E-03 4.520 14710.0 NC5H11OH+OH=C5H10OH11+H2O 3.610E+03 2.890 -2291.0 NC5H11OH+HO2=C5H1
3.500E-05 5.260 8268.0 NC5H11OH+OH=C5H11O-1+H2O 5.880E+02 2.820 -585.0 NC5H11OH+HO2=C5H11O-
1+H2O2 6.470E-07 5.300 10530.0 C5H10OH15=¿C2H4+C2H4+CH2OH 5.170E+13 0.103 29084.0
C3H6+PC2H4OH=C5H10OH14 8.800E+03 2.480 6130.0 C4H71-4OH+CH3=C5H10OH13 1.760E+04
2.480 6130.0 C4H8-1+CH2OH=C5H10OH13 8.800E+03 2.480 6130.0 C3H5OH+C2H5=C5H10OH12
8.800E+03 2.480 6130.0 C2H3OH+NC3H7=C5H10OH11 8.800E+03 2.480 6130.0 C5H10OH11+O2=C5H10OH-

1O2 5.000E+11 0.000 0.0 C5H10OH12+O2=C5H10OH-2O2 3.490E+14 -0.816 -536.0 C5H10OH13+O2=C5H10OH
3O2 3.490E+14 -0.816 -536.0 C5H10OH14+O2=C5H10OH-4O2 3.490E+14 -0.816 -536.0 C5H10OH15+O2=C5H1
5O2 6.860E+16 -1.627 199.0 C5H10OH-1O2=C5H9OH1-1+HO2 2.880E+09 0.930 29800.0 C5H10OH-
2O2=C5H9OH1-1+HO2 2.880E+09 0.930 29800.0 C5H10OH-2O2=C5H9OH1-2+HO2 2.880E+09
0.930 29800.0 C5H10OH-3O2=C5H9OH1-2+HO2 2.880E+09 0.930 29800.0 C5H10OH-3O2=C5H9OH1-
3+HO2 2.880E+09 0.930 29800.0 C5H10OH-4O2=C5H9OH1-3+HO2 2.880E+09 0.930 29800.0
C5H10OH-4O2=C5H9OH1-4+HO2 2.880E+09 0.930 29800.0 C5H10OH-5O2=C5H9OH1-4+HO2
2.880E+09 0.930 29800.0 C5H9OH1-1+OH=¿C4H7CHO-2+H+H2O 1.010E+06 2.200 -437.0 C5H9OH1-
2+OH=¿C4H7CHO-2+H+H2O 1.010E+06 2.200 -437.0 C5H9OH1-2+OH=¿C5H81-3+OH+H2O
1.010E+06 2.200 -437.0 C5H9OH1-3+OH=¿C5H81-3+OH+H2O 1.010E+06 2.200 -437.0 C5H9OH1-
4+OH=¿C4H6+CH2OH+H2O 1.010E+06 2.200 -437.0 NC6H14=CH3+C5H11-1 1.450E+51 -9.980
105372.0 PLOG / 1.00E-02 1.920E+94 -23.050 124349.0 / PLOG / 1.00E-01 7.100E+83 -19.750
121206.0 / PLOG / 1.00E+00 3.980E+68 -15.140 114401.0 / PLOG / 2.00E+00 2.520E+63 -13.590
111809.0 / PLOG / 5.00E+00 2.510E+56 -11.520 108177.0 / PLOG / 1.00E+01 1.450E+51 -9.980
105372.0 / PLOG / 2.00E+01 1.300E+46 -8.500 102608.0 / PLOG / 5.00E+01 8.780E+39 -6.700
99154.0 / NC6H14=C2H5+PC4H9 4.380E+52 -10.210 103971.0 PLOG / 1.00E-02 3.840E+96 -
23.490 123675.0 / PLOG / 1.00E-01 3.950E+85 -20.040 120116.0 / PLOG / 1.00E+00 1.160E+70
-15.350 113057.0 / PLOG / 2.00E+00 6.940E+64 -13.800 110428.0 / PLOG / 5.00E+00 7.030E+57
-11.740 106773.0 / PLOG / 1.00E+01 4.380E+52 -10.210 103971.0 / PLOG / 2.00E+01 4.450E+47
-8.740 101224.0 / PLOG / 5.00E+01 3.730E+41 -6.970 97811.0 / NC6H14=NC3H7+NC3H7
3.000E+54 -10.740 104866.0 PLOG / 1.00E-02 8.730E+97 -23.890 124152.0 / PLOG / 1.00E-
01 1.930E+87 -20.530 120839.0 / PLOG / 1.00E+00 8.220E+71 -15.890 113924.0 / PLOG /
2.00E+00 5.070E+66 -14.340 111315.0 / PLOG / 5.00E+00 5.060E+59 -12.270 107672.0 / PLOG
/ 1.00E+01 3.000E+54 -10.740 104866.0 / PLOG / 2.00E+01 2.820E+49 -9.260 102108.0 / PLOG
/ 5.00E+01 2.070E+43 -7.470 98669.0 / NC6H14=C6H13-1+H 9.880E+51 -10.510 119684.0 PLOG
/ 1.00E-02 1.140E+82 -20.070 128443.0 / PLOG / 1.00E-01 4.840E+78 -18.720 130156.0 / PLOG
/ 1.00E+00 1.570E+68 -15.390 127126.0 / PLOG / 2.00E+00 5.740E+63 -14.040 125268.0 /
PLOG / 5.00E+00 1.750E+57 -12.080 122267.0 / PLOG / 1.00E+01 9.880E+51 -10.510 119684.0
/ PLOG / 2.00E+01 4.440E+46 -8.930 116936.0 / PLOG / 5.00E+01 5.140E+39 -6.890 113232.0 /
NC6H14=C6H13-2+H 3.070E+51 -10.350 115970.0 PLOG / 1.00E-02 7.120E+85 -21.090 127902.0
/ PLOG / 1.00E-01 2.570E+80 -19.160 128267.0 / PLOG / 1.00E+00 2.050E+68 -15.390 124032.0
/ PLOG / 2.00E+00 3.710E+63 -13.950 121912.0 / PLOG / 5.00E+00 6.390E+56 -11.930 118663.0
/ PLOG / 1.00E+01 3.070E+51 -10.350 115970.0 / PLOG / 2.00E+01 1.460E+46 -8.780 113177.0
/ PLOG / 5.00E+01 2.410E+39 -6.790 109502.0 / NC6H14=C6H13-3+H 3.070E+51 -10.350
115970.0 PLOG / 1.00E-02 7.120E+85 -21.090 127902.0 / PLOG / 1.00E-01 2.570E+80 -19.160
128267.0 / PLOG / 1.00E+00 2.050E+68 -15.390 124032.0 / PLOG / 2.00E+00 3.710E+63 -

13.950 121912.0 / PLOG / 5.00E+00 6.390E+56 -11.930 118663.0 / PLOG / 1.00E+01 3.070E+51
-10.350 115970.0 / PLOG / 2.00E+01 1.460E+46 -8.780 113177.0 / PLOG / 5.00E+01 2.410E+39
-6.790 109502.0 / NC6H14+H=C6H13-1+H2 3.490E+05 2.690 6450.0 NC6H14+H=C6H13-2+H2
2.600E+06 2.400 4471.0 NC6H14+H=C6H13-3+H2 2.600E+06 2.400 4471.0 NC6H14+O=C6H13-
1+OH 1.130E+14 0.000 7850.0 NC6H14+O=C6H13-2+OH 5.620E+13 0.000 5200.0 NC6H14+O=C6H13-
3+OH 5.620E+13 0.000 5200.0 NC6H14+OH=C6H13-1+H2O 2.730E+07 1.813 868.0 NC6H14+OH=C6H13-
2+H2O 1.410E+10 0.935 505.0 NC6H14+OH=C6H13-3+H2O 1.140E+07 1.811 -1016.0 NC6H14+O2=C6H13-
1+HO2 4.200E+13 0.000 52800.0 NC6H14+O2=C6H13-2+HO2 2.800E+13 0.000 50160.0 NC6H14+O2=C6H13-
3+HO2 2.800E+13 0.000 50160.0 NC6H14+HO2=C6H13-1+H2O2 4.080E+01 3.590 17160.0 NC6H14+HO2=C6H
2+H2O2 1.896E+02 3.370 13720.0 NC6H14+HO2=C6H13-3+H2O2 1.896E+02 3.370 13720.0
NC6H14+CH3=C6H13-1+CH4 9.040E-01 3.650 7154.0 NC6H14+CH3=C6H13-2+CH4 3.020E+00
3.460 5481.0 NC6H14+CH3=C6H13-3+CH4 3.020E+00 3.460 5481.0 NC6H14+CH3O=C6H13-
1+CH3OH 4.340E+11 0.000 6458.0 NC6H14+CH3O=C6H13-2+CH3OH 2.900E+11 0.000 4571.0
NC6H14+CH3O=C6H13-3+CH3OH 2.900E+11 0.000 4571.0 NC6H14+CH3O2=C6H13-1+CH3O2H
1.390E+00 3.970 18280.0 NC6H14+CH3O2=C6H13-2+CH3O2H 2.040E+01 3.580 14810.0 NC6H14+CH3O2=C6H
3+CH3O2H 2.040E+01 3.580 14810.0 NC6H14+O2CHO=C6H13-1+HO2CHO 1.390E+00 3.970
18280.0 NC6H14+O2CHO=C6H13-2+HO2CHO 2.040E+01 3.580 14810.0 NC6H14+O2CHO=C6H13-
3+HO2CHO 2.040E+01 3.580 14810.0 NC6H14+C2H3=C6H13-1+C2H4 1.000E+12 0.000 18000.0
NC6H14+C2H3=C6H13-2+C2H4 8.000E+11 0.000 16800.0 NC6H14+C2H3=C6H13-3+C2H4 8.000E+11
0.000 16800.0 NC6H14+C2H5=C6H13-1+C2H6 1.000E+11 0.000 13400.0 NC6H14+C2H5=C6H13-
2+C2H6 1.000E+11 0.000 10400.0 NC6H14+C2H5=C6H13-3+C2H6 1.000E+11 0.000 10400.0
C6H13-1=C2H4+PC4H9 8.260E+12 0.200 28891.1 C6H13-2=C3H6+NC3H7 1.870E+12 0.410
28208.6 C6H13-3=C2H5+C4H8-1 9.430E+11 0.470 28238.3 C6H13-3=CH3+C5H10-1 3.110E+10
1.090 29769.5 C6H13-1+O2=C6H12-1+HO2 8.047E+00 3.320 12857.2 C6H13-2+O2=C6H12-1+HO2
2.645E+01 3.230 10591.8 C6H13-2+O2=C6H12-2+HO2 8.047E+00 3.320 12857.2 C6H13-3+O2=C6H12-
2+HO2 8.047E+00 3.320 12857.2 C6H13-3+O2=C6H12-3+HO2 8.047E+00 3.320 12857.2 C6H13-
2=C6H13-3 2.750E+10 0.700 41872.0 C6H13-1=C6H13-2 1.820E+02 2.550 10961.0 C6H13-1=C6H13-
3 6.920E+00 3.200 16559.0 C6H13-1+O2=C6H13O2-1 6.860E+16 -1.627 199.0 C6H13-2+O2=C6H13O2-
2 3.490E+14 -0.816 -536.0 C6H13-3+O2=C6H13O2-3 3.490E+14 -0.816 -536.0 C6H13-1+HO2=C6H13O-
1+OH 9.000E+12 0.000 -1000.0 C6H13-2+HO2=C6H13O-2+OH 9.000E+12 0.000 -1000.0 C6H13-
3+HO2=C6H13O-3+OH 9.000E+12 0.000 -1000.0 C6H13-1+CH3O2=C6H13O-1+CH3O 9.000E+12
0.000 -1000.0 C6H13-2+CH3O2=C6H13O-2+CH3O 9.000E+12 0.000 -1000.0 C6H13-3+CH3O2=C6H13O-
3+CH3O 9.000E+12 0.000 -1000.0 C6H13-1+C6H13O2-1=C6H13O-1+C6H13O-1 9.000E+12 0.000
-1000.0 C6H13-1+C6H13O2-2=C6H13O-1+C6H13O-2 9.000E+12 0.000 -1000.0 C6H13-1+C6H13O2-
3=C6H13O-1+C6H13O-3 9.000E+12 0.000 -1000.0 C6H13-2+C6H13O2-1=C6H13O-2+C6H13O-
1 9.000E+12 0.000 -1000.0 C6H13-2+C6H13O2-2=C6H13O-2+C6H13O-2 9.000E+12 0.000 -1000.0

C6H13-2+C6H13O2-3=C6H13O-2+C6H13O-3 9.000E+12 0.000 -1000.0 C6H13-3+C6H13O2-1=C6H13O-3+C6H13O-1 9.000E+12 0.000 -1000.0 C6H13-3+C6H13O2-2=C6H13O-3+C6H13O-2 9.000E+12 0.000 -1000.0 C6H13-3+C6H13O2-3=C6H13O-3+C6H13O-3 9.000E+12 0.000 -1000.0 C6H13O2-1=C6H12OOH1-2 4.010E+08 1.100 30100.0 C6H13O2-1=C6H12OOH1-3 1.360E+07 1.300 18200.0 C6H13O2-1=C6H12OOH1-4 3.720E+06 1.200 16600.0 C6H13O2-1=C6H12OOH1-5 2.600E+06 1.000 18200.0 C6H13O2-2=C6H12OOH2-1 2.110E+11 0.200 34200.0 C6H13O2-2=C6H12OOH2-3 1.720E+09 0.900 29500.0 C6H13O2-2=C6H12OOH2-4 7.030E+10 0.200 18500.0 C6H13O2-2=C6H12OOH2-5 3.720E+06 1.200 16600.0 C6H13O2-2=C6H12OOH2-6 1.470E+05 1.500 19900.0 C6H13O2-3=C6H12OOH3-1 1.440E+07 1.400 20800.0 C6H13O2-3=C6H12OOH3-2 1.720E+09 0.900 29500.0 C6H13O2-3=C6H12OOH3-4 1.720E+09 0.900 29500.0 C6H13O2-3=C6H12OOH3-5 7.030E+10 0.200 18500.0 C6H13O2-3=C6H12OOH3-6 1.230E+06 1.500 20000.0 C6H13O2-1=C6H12-1+HO2 3.870E+07 1.580 28500.0 C6H13O2-2=C6H12-1+HO2 3.605E+09 1.130 30600.0 C6H13O2-2=C6H12-2+HO2 6.168E+09 1.010 29362.0 C6H13O2-3=C6H12-2+HO2 6.168E+09 1.010 29362.0 C6H13O2-3=C6H12-3+HO2 6.168E+09 1.010 29362.0 C6H13OOH-1+O2=C6H13O2-1+HO2 3.750E+13 -0.800 33620.0 C6H13OOH-2+O2=C6H13O2-2+HO2 4.380E+13 -0.800 33640.0 C6H13OOH-3+O2=C6H13O2-3+HO2 4.380E+13 -0.800 33640.0 C6H13OOH-1+HO2=C6H13O2-1+H2O2 2.400E+12 0.000 10000.0 C6H13OOH-2+HO2=C6H13O2-2+H2O2 2.400E+12 0.000 10000.0 C6H13OOH-3+HO2=C6H13O2-3+H2O2 2.400E+12 0.000 10000.0 C6H13O2-1+NC6H14=C6H13OOH-1+C6H13-1 1.210E+13 0.000 20430.0 C6H13O2-1+NC6H14=C6H13OOH-1+C6H13-2 8.060E+12 0.000 17700.0 C6H13O2-1+NC6H14=C6H13OOH-1+C6H13-3 8.060E+12 0.000 17700.0 C6H13O2-2+NC6H14=C6H13OOH-2+C6H13-1 1.210E+13 0.000 20430.0 C6H13O2-2+NC6H14=C6H13OOH-2+C6H13-2 8.060E+12 0.000 17700.0 C6H13O2-2+NC6H14=C6H13OOH-2+C6H13-3 8.060E+12 0.000 17700.0 C6H13O2-3+NC6H14=C6H13OOH-3+C6H13-1 1.210E+13 0.000 20430.0 C6H13O2-3+NC6H14=C6H13OOH-3+C6H13-2 8.060E+12 0.000 17700.0 C6H13O2-3+NC6H14=C6H13OOH-3+C6H13-3 8.060E+12 0.000 17700.0 C6H13O2-1+CH3O2=¿C6H13O-1+CH3O+O2 1.400E+16 -1.600 1860.0 C6H13O2-2+CH3O2=¿C6H13O-2+CH3O+O2 1.400E+16 -1.600 1860.0 C6H13O2-3+CH3O2=¿C6H13O-3+CH3O+O2 1.400E+16 -1.600 1860.0 C6H13O2-1+C6H13O2-1=¿C6H13O-1+C6H13O-1+O2 1.400E+16 -1.600 1860.0 C6H13O2-1+C6H13O2-2=¿C6H13O-1+C6H13O-2+O2 1.400E+16 -1.600 1860.0 C6H13O2-1+C6H13O2-3=¿C6H13O-1+C6H13O-3+O2 1.400E+16 -1.600 1860.0 C6H13O2-2+C6H13O2-2=¿C6H13O-2+C6H13O-2+O2 1.400E+16 -1.600 1860.0 C6H13O2-2+C6H13O2-3=¿C6H13O-2+C6H13O-3+O2 1.400E+16 -1.600 1860.0 C6H13O2-3+C6H13O2-3=¿C6H13O-3+C6H13O-3+O2 1.400E+16 -1.600 1860.0 C6H13OOH-1=C6H13O-1+OH 1.500E+16 0.000 41600.0 C6H13OOH-2=C6H13O-2+OH 1.050E+16 0.000 41200.0 C6H13OOH-3=C6H13O-3+OH 1.050E+16 0.000 41200.0 C6H13O-1=CH2O+C5H11-1 2.000E+13 0.000 15000.0 C6H13O-2=CH3CHO+PC4H9 2.000E+13 0.000 15000.0 C6H13O-3=C2H5CHO+NC3H7 2.000E+13 0.000 15000.0 C6H12OOH1-2=C6H12O1-2+OH 3.550E+12 0.000 10714.0 C6H12OOH1-3=C6H12O1-3+OH 9.510E+11 0.000

16619.7 C6H12OOH1-4=C6H12O1-4+OH 2.770E+10 0.000 10501.1 C6H12OOH1-5=C6H12O1-5+OH 1.040E+10 0.000 11137.0 C6H12OOH2-1=C6H12O1-2+OH 3.550E+12 0.000 12371.9 C6H12OOH2-3=C6H12O2-3+OH 1.775E+12 0.000 12701.9 C6H12OOH2-4=C6H12O2-4+OH 6.340E+11 0.000 17612.1 C6H12OOH2-5=C6H12O2-5+OH 2.770E+10 0.000 11489.7 C6H12OOH2-6=C6H12O1-5+OH 1.040E+10 0.000 11907.9 C6H12OOH3-1=C6H12O1-3+OH 6.340E+11 0.000 17334.2 C6H12OOH3-2=C6H12O2-3+OH 1.775E+12 0.000 12701.9 C6H12OOH3-4=C6H12O3-4+OH 1.775E+12 0.000 12701.9 C6H12OOH3-5=C6H12O2-4+OH 6.340E+11 0.000 17612.1 C6H12OOH3-6=C6H12O1-4+OH 2.770E+10 0.000 11572.8 C6H12OOH1-2=C6H12-1+HO2 5.630E+09 0.970 15000.0 C6H12OOH2-1=C6H12-1+HO2 1.780E+12 0.240 15700.0 C6H12OOH2-3=C6H12-2+HO2 3.500E+11 0.370 14900.0 C6H12OOH3-2=C6H12-2+HO2 3.500E+11 0.370 14900.0 C6H12OOH3-4=C6H12-3+HO2 3.500E+11 0.370 14900.0 C6H12OOH1-3=¿CH2O+C5H10-1+OH 3.081E+13 0.000 27351.9 C6H12OOH2-4=¿CH3CHO+C4H8-1+OH 3.081E+13 0.000 24909.5 C6H12OOH3-1=¿NC3H7CHO+C2H4+OH 3.081E+13 0.000 24615.5 C6H12OOH3-5=¿C2H5CHO+C3H6+OH 3.081E+13 0.000 25551.9 C6H12OOH1-4=C2H4O2H+C4H8-1 1.392E+14 0.000 28090.0 C6H12OOH2-5=C3H6OOH2-1+C3H6 1.392E+14 0.000 29612.2 C6H12OOH3-6=C4H8OOH2-1+C2H4 1.392E+14 0.000 28136.4 C6H12OOH1-2+O2=C6H12OOH1-2O2 1.740E+14 -0.816 -536.0 C6H12OOH1-3+O2=C6H12OOH1-3O2 1.740E+14 -0.816 -536.0 C6H12OOH1-4+O2=C6H12OOH1-4O2 1.740E+14 -0.816 -536.0 C6H12OOH1-5+O2=C6H12OOH1-5O2 1.740E+14 -0.816 -536.0 C6H12OOH2-1+O2=C6H12OOH2-1O2 3.430E+16 -1.627 199.0 C6H12OOH2-3+O2=C6H12OOH2-3O2 1.740E+14 -0.816 -536.0 C6H12OOH2-4+O2=C6H12OOH2-4O2 1.740E+14 -0.816 -536.0 C6H12OOH2-5+O2=C6H12OOH2-5O2 1.740E+14 -0.816 -536.0 C6H12OOH2-6+O2=C6H12OOH2-6O2 3.430E+16 -1.627 199.0 C6H12OOH3-1+O2=C6H12OOH3-1O2 3.430E+16 -1.627 199.0 C6H12OOH3-2+O2=C6H12OOH3-2O2 1.740E+14 -0.816 -536.0 C6H12OOH3-4+O2=C6H12OOH3-4O2 1.740E+14 -0.816 -536.0 C6H12OOH3-5+O2=C6H12OOH3-5O2 1.740E+14 -0.816 -536.0 C6H12OOH3-6+O2=C6H12OOH3-6O2 3.430E+16 -1.627 199.0 C6H12OOH1-2O2=C6H11-2D1OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-3O2=C6H11-2D1OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-3O2=C6H11-3D1OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-4O2=C6H11-3D1OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-4O2=C6H11-2D6OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-5O2=C6H11-2D6OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH1-5O2=C6H11-1D6OOH+HO2 3.605E+09 1.130 30600.0 C6H12OOH2-3O2=C6H11-3D2OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH2-4O2=C6H11-3D2OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH2-4O2=C6H11-2D5OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH2-5O2=C6H11-2D5OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH2-5O2=C6H11-1D5OOH+HO2 3.605E+09 1.130 30600.0 C6H12OOH2-6O2=C6H11-1D5OOH+HO2 3.870E+07 1.580 28500.0 C6H12OOH3-1O2=C6H11-1D3OOH+HO2 3.870E+07 1.580 28500.0 C6H12OOH3-2O2=C6H11-1D3OOH+HO2 3.605E+09 1.130 30600.0 C6H12OOH3-4O2=C6H11-2D4OOH+HO2 6.168E+09 1.010 29362.0 C6H12OOH3-5O2=C6H11-2D4OOH+HO2 6.168E+09

1.010 29362.0 C6H12OOH3-5O2=C6H11-1D4OOH+HO2 3.605E+09 1.130 30600.0 C6H12OOH3-6O2=C6H11-1D4OOH+HO2 3.870E+07 1.580 28500.0 C6H12OOH1-2O2=C6H11Q12-3 1.720E+09 0.900 29500.0 C6H12OOH1-2O2=C6H11Q12-4 7.030E+10 0.200 18500.0 C6H12OOH1-2O2=C6H11Q12-5 3.720E+06 1.200 16600.0 C6H12OOH1-2O2=C6H11Q12-6 1.470E+05 1.500 19900.0 C6H12OOH1-3O2=C6H11Q13-2 1.720E+09 0.900 29500.0 C6H12OOH1-3O2=C6H11Q13-4 1.720E+09 0.900 29500.0 C6H12OOH1-3O2=C6H11Q13-5 7.030E+10 0.200 18500.0 C6H12OOH1-3O2=C6H11Q13-6 6.170E+05 1.500 20000.0 C6H12OOH1-4O2=C6H11Q14-2 7.030E+10 0.200 18500.0 C6H12OOH1-4O2=C6H11Q14-3 1.720E+09 0.900 29500.0 C6H12OOH1-4O2=C6H11Q14-5 1.720E+09 0.900 29500.0 C6H12OOH1-4O2=C6H11Q14-6 1.440E+07 1.400 20800.0 C6H12OOH1-5O2=C6H11Q15-2 3.720E+06 1.200 16600.0 C6H12OOH1-5O2=C6H11Q15-3 7.030E+10 0.200 18500.0 C6H12OOH1-5O2=C6H11Q15-4 1.720E+09 0.900 29500.0 C6H12OOH1-5O2=C6H11Q15-6 2.110E+11 0.200 34200.0 C6H12OOH2-1O2=C6H11Q12-3 1.360E+07 1.300 18200.0 C6H12OOH2-1O2=C6H11Q12-4 3.720E+06 1.200 16600.0 C6H12OOH2-1O2=C6H11Q12-5 2.600E+06 1.000 18200.0 C6H12OOH2-3O2=C6H11Q23-1 1.440E+07 1.400 20800.0 C6H12OOH2-3O2=C6H11Q23-4 1.720E+09 0.900 29500.0 C6H12OOH2-3O2=C6H11Q23-5 7.030E+10 0.200 18500.0 C6H12OOH2-3O2=C6H11Q23-6 6.170E+05 1.500 20000.0 C6H12OOH2-4O2=C6H11Q24-1 6.170E+05 1.500 20000.0 C6H12OOH2-4O2=C6H11Q24-3 1.720E+09 0.900 29500.0 C6H12OOH2-4O2=C6H11Q24-5 1.720E+09 0.900 29500.0 C6H12OOH2-4O2=C6H11Q24-6 1.440E+07 1.400 20800.0 C6H12OOH2-5O2=C6H11Q25-1 1.470E+05 1.500 19900.0 DUP C6H12OOH2-5O2=C6H11Q25-3 7.030E+10 0.200 18500.0 DUP C6H12OOH2-5O2=C6H11Q25-3 1.720E+09 0.900 29500.0 DUP C6H12OOH2-5O2=C6H11Q25-1 2.110E+11 0.200 34200.0 DUP C6H12OOH2-6O2=C6H11Q15-4 3.720E+06 1.200 16600.0 C6H12OOH2-6O2=C6H11Q15-3 1.360E+07 1.300 18200.0 C6H12OOH2-6O2=C6H11Q15-2 4.010E+08 1.100 30100.0 C6H12OOH3-1O2=C6H11Q13-2 4.010E+08 1.100 30100.0 C6H12OOH3-1O2=C6H11Q13-4 3.720E+06 1.200 16600.0 C6H12OOH3-1O2=C6H11Q13-5 2.600E+06 1.000 18200.0 C6H12OOH3-2O2=C6H11Q23-1 2.110E+11 0.200 34200.0 C6H12OOH3-2O2=C6H11Q23-4 7.030E+10 0.200 18500.0 C6H12OOH3-2O2=C6H11Q23-5 3.720E+06 1.200 16600.0 C6H12OOH3-2O2=C6H11Q23-6 1.470E+05 1.500 19900.0 C6H12OOH3-4O2=C6H11Q34-1 6.170E+05 1.500 20000.0 DUP C6H12OOH3-4O2=C6H11Q34-2 7.030E+10 0.200 18500.0 DUP C6H12OOH3-4O2=C6H11Q34-2 1.720E+09 0.900 29500.0 DUP C6H12OOH3-4O2=C6H11Q34-1 1.440E+07 1.400 20800.0 DUP C6H12OOH3-5O2=C6H11Q24-6 1.470E+05 1.500 19900.0 C6H12OOH3-5O2=C6H11Q24-5 3.720E+06 1.200 16600.0 C6H12OOH3-5O2=C6H11Q24-3 1.720E+09 0.900 29500.0 C6H12OOH3-5O2=C6H11Q24-1 2.110E+11 0.200 34200.0 C6H12OOH3-6O2=C6H11Q14-5 2.600E+06 1.000 18200.0 C6H12OOH3-6O2=C6H11Q14-3 1.360E+07 1.300 18200.0 C6H12OOH3-6O2=C6H11Q14-2 4.010E+08 1.100 30100.0 C6H12OOH1-2O2=C6KET12+OH 2.440E+07 1.600 27900.0 C6H12OOH1-3O2=C6KET13+OH 1.100E+04 2.400 19900.0 C6H12OOH1-4O2=C6KET14+OH 1.260E+03 2.200 17400.0 C6H12OOH1-5O2=C6KET15+OH 1.110E+03 1.800 16600.0 C6H12OOH2-1O2=C6KET21+OH 2.760E+08 1.200

25700.0 C6H12OOH2-3O2=C6KET23+OH 1.750E+08 1.700 26000.0 C6H12OOH2-4O2=C6KET24+OH
1.750E+02 3.100 17500.0 C6H12OOH2-5O2=C6KET25+OH 2.540E+02 2.600 16200.0 C6H12OOH2-
6O2=C6KET26+OH 2.000E+03 1.900 14900.0 C6H12OOH3-1O2=C6KET31+OH 5.790E+01 2.900
17000.0 C6H12OOH3-2O2=C6KET32+OH 1.750E+08 1.700 26000.0 C6H12OOH3-4O2=C6KET34+OH
1.750E+08 1.700 26000.0 C6H12OOH3-5O2=C6KET35+OH 1.750E+02 3.100 17500.0 C6H12OOH3-
6O2=C6KET36+OH 3.770E+02 2.200 15300.0 C6H11Q12-4=¿C4H8-1+HO2CH2CHO+OH 3.081E+13
0.000 26826.0 C6H11Q13-5=¿C3KET13+C3H6+OH 3.081E+13 0.000 24963.6 C6H11Q14-6=¿NC4KET14+C2H4+
3.081E+13 0.000 24615.6 C6H11Q15-3=¿C4H71-4OOH+CH3CHO+OH 3.081E+13 0.000 24909.5
C6H11Q15-3=¿C5H91-4OOH+CH2O+OH 3.081E+13 0.000 27330.7 C6H11Q23-5=¿C3KET12+C3H6+OH
3.081E+13 0.000 24719.9 C6H11Q24-6=¿NC4KET13+C2H4+OH 3.081E+13 0.000 24615.6 C6H11Q34-
1=¿NC4KET12+C2H4+OH 3.081E+13 0.000 26370.1 C6H11Q12-5=C3H51-2,3OOH+C3H6 1.392E+14
0.000 27231.1 C6H11Q13-6=C4H71-2,4OOH+C2H4 1.392E+14 0.000 28136.5 C6H11Q23-6=C4H71-
2,3OOH+C2H4 1.392E+14 0.000 28136.4 C6KET12=C6KET12O+OH 1.050E+16 0.000 41800.0
C6KET13=C6KET13O+OH 1.050E+16 0.000 41800.0 C6KET14=C6KET14O+OH 1.050E+16 0.000
41800.0 C6KET15=C6KET15O+OH 1.050E+16 0.000 41800.0 C6KET21=C6KET21O+OH 1.500E+16
0.000 40800.0 C6KET23=C6KET23O+OH 1.050E+16 0.000 41800.0 C6KET24=C6KET24O+OH
1.050E+16 0.000 41800.0 C6KET25=C6KET25O+OH 1.050E+16 0.000 41800.0 C6KET26=C6KET26O+OH
1.500E+16 0.000 40800.0 C6KET31=C6KET31O+OH 1.500E+16 0.000 40800.0 C6KET32=C6KET32O+OH
1.050E+16 0.000 41800.0 C6KET34=C6KET34O+OH 1.050E+16 0.000 41800.0 C6KET35=C6KET35O+OH
1.050E+16 0.000 41800.0 C6KET36=C6KET36O+OH 1.500E+16 0.000 40800.0 C6KET12O=PC4H9CHO+HCO
2.900E+12 0.400 11080.0 C6KET13O=NC3H7CHO+CH2CHO 2.900E+12 0.400 11080.0 C6KET14O=C2H5CHO+
2.900E+12 0.400 11080.0 C6KET15O=CH3CHO+C3H6CHO-1 2.900E+12 0.400 11080.0 C6KET21O=CH2O+PC4
2.900E+12 0.400 11080.0 C6KET23O=NC3H7CHO+CH3CO 2.900E+12 0.400 11080.0 C6KET24O=C2H5CHO+C
2.900E+12 0.400 11080.0 C6KET25O=CH3CHO+CH2CH2COCH3 2.900E+12 0.400 11080.0 C6KET26O=CH2O+
2.900E+12 0.400 11080.0 C6KET31O=CH2O+NC3H7COCH2 2.900E+12 0.400 11080.0 C6KET32O=CH3CHO+N
2.900E+12 0.400 11080.0 C6KET34O=C2H5CHO+C2H5CO 2.900E+12 0.400 11080.0 C6KET35O=CH3CHO+C2H
2.900E+12 0.400 11080.0 C6KET36O=CH2O+CH2CH2COC2H5 2.900E+12 0.400 11080.0 C6H11Q12-
3=C6H11-2D1OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q13-2=C6H11-1D3OOH+HO2 5.630E+09
0.970 15000.0 C6H11Q13-2=C6H11-2D1OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q13-4=C6H11-
3D1OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q14-2=C6H11-1D4OOH+HO2 5.630E+09 0.970
15000.0 C6H11Q14-3=C6H11-3D1OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q14-5=C6H11-
2D6OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q15-2=C6H11-1D5OOH+HO2 5.630E+09 0.970
15000.0 C6H11Q15-4=C6H11-2D6OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q15-6=C6H11-
1D6OOH+HO2 1.780E+12 0.240 15700.0 C6H11Q23-1=C6H11-1D3OOH+HO2 5.630E+09 0.970
15000.0 C6H11Q23-4=C6H11-3D2OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q24-1=C6H11-
1D4OOH+HO2 1.780E+12 0.240 15700.0 C6H11Q24-3=C6H11-2D4OOH+HO2 3.500E+11 0.370

14900.0 C6H11Q24-3=C6H11-3D2OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q24-5=C6H11-2D5OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q25-1=C6H11-1D5OOH+HO2 5.630E+09 0.970 15000.0 C6H11Q25-3=C6H11-2D5OOH+HO2 3.500E+11 0.370 14900.0 C6H11Q34-2=C6H11-2D4OOH+HO2 3.500E+11 0.370 14900.0 C6H11-1D3OOH=¿C2H3CHO+NC3H7+OH 1.050E+16 0.000 41800.0 C6H11-1D4OOH=¿AC3H5CHO+C2H5+OH 1.050E+16 0.000 41800.0 C6H11-1D4OOH=¿C3H5-A+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11-1D5OOH=¿C4H71-4+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11-1D6OOH=¿C5H91-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11-2D1OOH=¿C5H91-1+CH2O+OH 1.050E+16 0.000 40800.0 C6H11-2D4OOH=¿SC3H5CHO+C2H5+OH 1.050E+16 0.000 41800.0 C6H11-2D4OOH=¿C3H5-S+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11-2D6OOH=¿C5H92-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11-3D1OOH=¿C5H91-3+CH2O+OH 1.500E+16 0.000 40800.0 C6H11-3D2OOH=¿CH3CHO+C4H71-1+OH 1.500E+16 0.000 41800.0 C2H2+NC3H7=C5H91-1 2.000E+11 0.000 7800.0 C6H11Q12-3=C6H11O13-2OOH+OH 9.510E+11 0.000 16330.9 C6H11Q12-3=C6H11O23-1OOH+OH 1.775E+12 0.000 12701.9 C6H11Q12-4=C6H11O14-2OOH+OH 2.770E+10 0.000 10501.1 C6H11Q12-4=C6H11O24-1OOH+OH 6.340E+11 0.000 17612.1 C6H11Q12-5=C6H11O15-2OOH+OH 1.040E+10 0.000 11137.0 C6H11Q12-5=C6H11O25-1OOH+OH 2.770E+10 0.000 11489.7 C6H11Q12-6=C6H11O15-6OOH+OH 1.040E+10 0.000 11907.9 C6H11Q13-2=C6H11O12-3OOH+OH 3.550E+12 0.000 10714.0 C6H11Q13-2=C6H11O23-1OOH+OH 1.775E+12 0.000 12701.9 C6H11Q13-4=C6H11O14-3OOH+OH 2.770E+10 0.000 10067.8 C6H11Q13-4=C6H11O34-1OOH+OH 1.775E+12 0.000 12701.9 C6H11Q13-5=C6H11O15-3OOH+OH 1.040E+10 0.000 11137.0 C6H11Q13-5=C6H11O24-6OOH+OH 6.340E+11 0.000 17612.1 C6H11Q13-6=C6H11O14-6OOH+OH 2.770E+10 0.000 11572.8 C6H11Q14-2=C6H11O12-4OOH+OH 3.550E+12 0.000 10714.0 C6H11Q14-2=C6H11O24-1OOH+OH 6.340E+11 0.000 17323.3 C6H11Q14-3=C6H11O13-4OOH+OH 9.510E+11 0.000 16330.9 C6H11Q14-3=C6H11O34-1OOH+OH 1.775E+12 0.000 12701.9 C6H11Q14-5=C6H11O15-4OOH+OH 1.040E+10 0.000 10825.4 C6H11Q14-5=C6H11O23-6OOH+OH 1.775E+12 0.000 12701.9 C6H11Q14-6=C6H11O13-6OOH+OH 6.340E+11 0.000 17334.2 C6H11Q15-2=C6H11O12-5OOH+OH 3.550E+12 0.000 10714.0 C6H11Q15-2=C6H11O25-1OOH+OH 2.770E+10 0.000 11056.4 C6H11Q15-3=C6H11O13-5OOH+OH 9.510E+11 0.000 16619.7 C6H11Q15-3=C6H11O24-6OOH+OH 6.340E+11 0.000 17612.1 C6H11Q15-4=C6H11O14-5OOH+OH 2.770E+10 0.000 10067.8 C6H11Q15-4=C6H11O23-6OOH+OH 1.775E+12 0.000 12701.9 C6H11Q15-6=C6H11O12-6OOH+OH 3.550E+12 0.000 12371.9 C6H11Q23-1=C6H11O12-3OOH+OH 3.550E+12 0.000 12371.9 C6H11Q23-1=C6H11O13-2OOH+OH 6.340E+11 0.000 17372.2 C6H11Q23-4=C6H11O24-3OOH+OH 6.340E+11 0.000 17323.3 C6H11Q23-4=C6H11O34-2OOH+OH 1.775E+12 0.000 12701.9 C6H11Q23-5=C6H11O25-3OOH+OH 2.770E+10 0.000 11489.7 C6H11Q23-5=C6H11O24-5OOH+OH 6.340E+11 0.000 17612.1 C6H11Q23-6=C6H11O15-4OOH+OH 1.040E+10 0.000 11907.9 C6H11Q23-6=C6H11O14-5OOH+OH 2.770E+10 0.000 11572.8 C6H11Q24-1=C6H11O12-4OOH+OH 3.550E+12 0.000 12371.9 C6H11Q24-1=C6H11O14-2OOH+OH 2.770E+10 0.000 11629.8 C6H11Q24-3=C6H11O23-4OOH+OH 1.775E+12 0.000 12701.9 C6H11Q24-3=C6H11O34-2OOH+OH

1.775E+12 0.000 12701.9 C6H11Q24-5=C6H11O25-3OOH+OH 2.770E+10 0.000 11056.4 C6H11Q24-5=C6H11O23-5OOH+OH 1.775E+12 0.000 12701.9 C6H11Q24-6=C6H11O15-3OOH+OH 1.040E+10 0.000 11907.9 C6H11Q24-6=C6H11O13-5OOH+OH 6.340E+11 0.000 17334.2 C6H11Q25-1=C6H11O12-5OOH+OH 3.550E+12 0.000 12371.9 C6H11Q25-1=C6H11O15-2OOH+OH 1.040E+10 0.000 11948.9 C6H11Q25-3=C6H11O23-5OOH+OH 1.775E+12 0.000 12701.9 C6H11Q25-3=C6H11O24-5OOH+OH 6.340E+11 0.000 17323.3 C6H11Q34-1=C6H11O13-4OOH+OH 6.340E+11 0.000 17334.2 C6H11Q34-1=C6H11O14-3OOH+OH 2.770E+10 0.000 11572.8 C6H11Q34-2=C6H11O23-4OOH+OH 1.775E+12 0.000 12701.9 C6H11Q34-2=C6H11O24-3OOH+OH 6.340E+11 0.000 17323.3 C6H11O12-3OOH=¿CH2CHO+NC
1.050E+16 0.000 41800.0 C6H11O12-4OOH=¿C3H5O+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11O12-5OOH=¿C4H7O12-4+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O12-6OOH=¿C5H9O12-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O13-2OOH=¿CH2CHO+NC3H7CHO+OH 1.050E+16 0.000 41800.0 C6H11O13-4OOH=¿CH2CH2CHO+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11O13-5OOH=¿C4H7O13-4+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O13-6OOH=¿C5H9O13-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O14-2OOH=¿CH2O+PC4H8CHO-2+OH 1.500E+16 0.000 41800.0 C6H11O14-3OOH=¿CH2CH2CHO+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11O14-5OOH=¿C3H6CHO-1+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O14-6OOH=¿C5H9O14-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O15-2OOH=¿CH2O+PC4H8CHO-3+OH 1.500E+16 0.000 41800.0 C6H11O15-3OOH=¿C3H6+CH2CHO+CH2O+OH 1.050E+16 0.000 41800.0 C6H11O15-4OOH=¿C3H6CHO-1+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O15-6OOH=¿PC4H8CHO-4+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O23-1OOH=¿CH2O+PC4H8CHO-1+OH 1.500E+16 0.000 40800.0 C6H11O23-4OOH=¿CH3CHCHO+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11O23-5OOH=¿C4H7O23-1+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O23-6OOH=¿C5H9O23-5+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O24-1OOH=¿CH2O+PC4H8CHO-2+OH 1.500E+16 0.000 40800.0 C6H11O24-3OOH=¿CH3CHCHO+C2H5CHO+OH 1.050E+16 0.000 41800.0 C6H11O24-5OOH=¿C3H6CHO-2+CH3CHO+OH 1.050E+16 0.000 41800.0 C6H11O24-6OOH=¿C5H9O24-1+CH2O+OH 1.500E+16 0.000 40800.0 C6H11O25-1OOH=¿CH2O+PC4H8CHO-3+OH 1.500E+16 0.000 40800.0 C6H11O25-3OOH=¿CH3CHO+C3H6CHO-2+OH 1.050E+16 0.000 41800.0 C6H11O34-1OOH=¿CH2O+C5H9O23-1+OH 1.500E+16 0.000 40800.0 C6H11O34-2OOH=¿CH3CHO+C3H6CHO-3+OH 1.050E+16 0.000 41800.0 C6H12O1-2+OH=¿CH2CO+PC4H9+H2O 2.500E+12 0.000 0.0 C6H12O1-2+OH=¿C2H3CHO+NC3H7+
2.500E+12 0.000 0.0 C6H12O1-3+OH=¿C2H4+NC3H7CO+H2O 2.500E+12 0.000 0.0 C6H12O1-3+OH=¿HCO+C5H10-1+H2O 2.500E+12 0.000 0.0 C6H12O1-4+OH=¿C2H4+C2H5COCH2+H2O 2.500E+12 0.000 0.0 C6H12O1-4+OH=¿CH2CHO+C4H8-1+H2O 2.500E+12 0.000 0.0 C6H12O1-5+OH=¿C2H4+CH2CH2COCH3+H2O 2.500E+12 0.000 0.0 C6H12O1-5+OH=¿CH2CH2CHO+C3H6+H2O 2.500E+12 0.000 0.0 C6H12O2-3+OH=¿C2H3COCH3+C2H5+H2O 2.500E+12 0.000 0.0 C6H12O2-3+OH=¿CH3CHCO+NC3H7+H2O 2.500E+12 0.000 0.0 C6H12O2-4+OH=¿C4H8-1+CH3CO+H2O 2.500E+12 0.000 0.0 C6H12O2-4+OH=¿C2H5CO+C3H6+H2O 2.500E+12 0.000 0.0 C6H12O2-

5+OH=¿C3H6+CH3COCH2+H2O 5.000E+12 0.000 0.0 C6H12O3-4+OH=¿C2H5+C2H5CHCO+H2O
5.000E+12 0.000 0.0 C6H12O1-2+HO2=¿CH2CO+PC4H9+H2O2 5.000E+12 0.000 17700.0 C6H12O1-
2+HO2=¿C2H3CHO+NC3H7+H2O2 5.000E+12 0.000 17700.0 C6H12O1-3+HO2=¿C2H4+NC3H7CO+H2O2
5.000E+12 0.000 17700.0 C6H12O1-3+HO2=¿HCO+C5H10-1+H2O2 5.000E+12 0.000 17700.0
C6H12O1-4+HO2=¿C2H4+C2H5COCH2+H2O2 5.000E+12 0.000 17700.0 C6H12O1-4+HO2=¿CH2CHO+C4H8-
1+H2O2 5.000E+12 0.000 17700.0 C6H12O1-5+HO2=¿C2H4+CH2CH2COCH3+H2O2 5.000E+12
0.000 17700.0 C6H12O1-5+HO2=¿CH2CH2CHO+C3H6+H2O2 5.000E+12 0.000 17700.0 C6H12O2-
3+HO2=¿C2H3COCH3+C2H5+H2O2 5.000E+12 0.000 17700.0 C6H12O2-3+HO2=¿CH3CHCO+NC3H7+H2O2
5.000E+12 0.000 17700.0 C6H12O2-4+HO2=¿C4H8-1+CH3CO+H2O2 5.000E+12 0.000 17700.0
C6H12O2-4+HO2=¿C2H5CO+C3H6+H2O2 5.000E+12 0.000 17700.0 C6H12O2-5+HO2=¿C3H6+CH3COCH2+H
1.000E+13 0.000 17700.0 C6H12O3-4+HO2=¿C2H5+C2H5CHCO+H2O2 1.000E+13 0.000 17700.0
CH3COOH=CH4+CO2 1.500E+13 0.000 70000.0 CH3COOH=H2O+CH2CO 1.400E+12 0.000
65000.0 CH3COOH=¿CO+OH+CH3 7.500E+15 0.000 91600.0 CH3COOH=¿CH3+CO2+H 2.500E+14
0.000 88000.0 C2H5COOH=¿C2H6+CO2 1.500E+13 0.000 70000.0 C2H5COOH=¿H2O+CH3CHCO
1.400E+12 0.000 65000.0 C2H5COOH=¿CO+OH+C2H5 7.500E+15 0.000 91600.0 C2H5COOH=¿CO2+C2H5+H
2.500E+14 0.000 88000.0 C6H13O2-1+CH3=C6H13O-1+CH3O 9.000E+12 0.000 -1000.0 C6H13O2-
2+CH3=C6H13O-2+CH3O 9.000E+12 0.000 -1000.0 C6H13O2-3+CH3=C6H13O-3+CH3O 9.000E+12
0.000 -1000.0 C6H13O2-1+C2H5=C6H13O-1+C2H5O 9.000E+12 0.000 -1000.0 C6H13O2-2+C2H5=C6H13O-
2+C2H5O 9.000E+12 0.000 -1000.0 C6H13O2-3+C2H5=C6H13O-3+C2H5O 9.000E+12 0.000 -
1000.0 C6H12OOH1-2O2+CH3=¿CH3O+C6H12OOH1-2O 9.000E+12 0.000 -1000.0 C6H12OOH1-
3O2+CH3=¿CH3O+C6H12OOH1-3O 9.000E+12 0.000 -1000.0 C6H12OOH1-4O2+CH3=¿CH3O+C6H12OOH1-
4O 9.000E+12 0.000 -1000.0 C6H12OOH1-5O2+CH3=¿CH3O+C6H12OOH1-5O 9.000E+12 0.000
-1000.0 C6H12OOH2-1O2+CH3=¿CH3O+C6H12OOH2-1O 9.000E+12 0.000 -1000.0 C6H12OOH2-
3O2+CH3=¿CH3O+C6H12OOH2-3O 9.000E+12 0.000 -1000.0 C6H12OOH2-4O2+CH3=¿CH3O+C6H12OOH2-
4O 9.000E+12 0.000 -1000.0 C6H12OOH2-5O2+CH3=¿CH3O+C6H12OOH2-5O 9.000E+12 0.000
-1000.0 C6H12OOH2-6O2+CH3=¿CH3O+C6H12OOH2-6O 9.000E+12 0.000 -1000.0 C6H12OOH3-
1O2+CH3=¿CH3O+C6H12OOH3-1O 9.000E+12 0.000 -1000.0 C6H12OOH3-2O2+CH3=¿CH3O+C6H12OOH3-
2O 9.000E+12 0.000 -1000.0 C6H12OOH3-4O2+CH3=¿CH3O+C6H12OOH3-4O 9.000E+12 0.000
-1000.0 C6H12OOH3-5O2+CH3=¿CH3O+C6H12OOH3-5O 9.000E+12 0.000 -1000.0 C6H12OOH3-
6O2+CH3=¿CH3O+C6H12OOH3-6O 9.000E+12 0.000 -1000.0 C6H12OOH1-2O=¿HO2CH2CHO+PC4H9
2.900E+12 0.400 11080.0 C6H12OOH1-3O=¿C3KET13+NC3H7 2.900E+12 0.400 11080.0 C6H12OOH1-
4O=¿NC4KET14+C2H5 2.900E+12 0.400 11080.0 C6H12OOH1-5O=¿NC5KET15+CH3 2.900E+12
0.400 11080.0 C6H12OOH2-1O=¿CH2O+PC4H9CHO+OH 2.900E+12 0.400 11080.0 C6H12OOH2-
3O=¿C3KET12+NC3H7 2.900E+12 0.400 11080.0 C6H12OOH2-4O=¿NC4KET13+C2H5 2.900E+12
0.400 11080.0 C6H12OOH2-5O=¿NC5KET14+CH3 2.900E+12 0.400 11080.0 C6H12OOH2-6O=¿CH2O+C5H10O
5 2.900E+12 0.400 11080.0 C6H12OOH3-1O=¿CH2O+C5H10OOH2-1 2.900E+12 0.400 11080.0

C6H12OOH3-2O=¿CH3+NC5KET12 2.900E+12 0.400 11080.0 C6H12OOH3-4O=¿NC4KET12+C2H5 2.900E+12 0.400 11080.0 C6H12OOH3-5O=¿CH3+NC5KET13 2.900E+12 0.400 11080.0 C6H12OOH3-6O=¿CH2O+C5H10OOH3-1 2.900E+12 0.400 11080.0 C6H12OOH1-2O=¿CH2O2H+PC4H9CHO 2.900E+12 0.400 11080.0 C6H12OOH1-3O=¿C2H4O2H+NC3H7CHO 2.900E+12 0.400 11080.0 C6H12OOH1-4O=¿C3H6OOH1-3+C2H5CHO 2.900E+12 0.400 11080.0 C6H12OOH1-5O=¿C4H8OOH1-4+CH3CHO 2.900E+12 0.400 11080.0 C6H12OOH2-3O=¿CH3CHO+NC3H7CHO+OH 2.900E+12 0.400 11080.0 C6H12OOH2-4O=¿C3H6OOH2-1+C2H5CHO 2.900E+12 0.400 11080.0 C6H12OOH2-5O=¿C4H8OOH2-4+CH3CHO 2.900E+12 0.400 11080.0 C6H12OOH3-2O=¿CH3CHO+NC3H7CHO+OH 2.900E+12 0.400 11080.0 C6H12OOH3-4O=¿C2H5CHO+C2H5CHO+OH 2.900E+12 0.400 11080.0 C6H12OOH3-5O=¿C4H8OOH2-1+CH3CHO 2.900E+12 0.400 11080.0 C6H12OOH1-2O2+C6H13-1=¿C6H13O-1+C6H12OOH1-2O 9.000E+12 0.000 -1000.0 C6H12OOH1-3O2+C6H13-1=¿C6H13O-1+C6H12OOH1-3O 9.000E+12 0.000 -1000.0 C6H12OOH1-4O2+C6H13-1=¿C6H13O-1+C6H12OOH1-4O 9.000E+12 0.000 -1000.0 C6H12OOH1-5O2+C6H13-1=¿C6H13O-1+C6H12OOH1-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-1O2+C6H13-1=¿C6H13O-1+C6H12OOH2-1O 9.000E+12 0.000 -1000.0 C6H12OOH2-3O2+C6H13-1=¿C6H13O-1+C6H12OOH2-3O 9.000E+12 0.000 -1000.0 C6H12OOH2-4O2+C6H13-1=¿C6H13O-1+C6H12OOH2-4O 9.000E+12 0.000 -1000.0 C6H12OOH2-5O2+C6H13-1=¿C6H13O-1+C6H12OOH2-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-6O2+C6H13-1=¿C6H13O-1+C6H12OOH2-6O 9.000E+12 0.000 -1000.0 C6H12OOH3-1O2+C6H13-1=¿C6H13O-1+C6H12OOH3-1O 9.000E+12 0.000 -1000.0 C6H12OOH3-2O2+C6H13-1=¿C6H13O-1+C6H12OOH3-2O 9.000E+12 0.000 -1000.0 C6H12OOH3-4O2+C6H13-1=¿C6H13O-1+C6H12OOH3-4O 9.000E+12 0.000 -1000.0 C6H12OOH3-5O2+C6H13-1=¿C6H13O-1+C6H12OOH3-5O 9.000E+12 0.000 -1000.0 C6H12OOH3-6O2+C6H13-1=¿C6H13O-1+C6H12OOH3-6O 9.000E+12 0.000 -1000.0 C6H12OOH1-2O2+C6H13-2=¿C6H13O-2+C6H12OOH1-2O 9.000E+12 0.000 -1000.0 C6H12OOH1-3O2+C6H13-2=¿C6H13O-2+C6H12OOH1-3O 9.000E+12 0.000 -1000.0 C6H12OOH1-4O2+C6H13-2=¿C6H13O-2+C6H12OOH1-4O 9.000E+12 0.000 -1000.0 C6H12OOH1-5O2+C6H13-2=¿C6H13O-2+C6H12OOH1-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-1O2+C6H13-2=¿C6H13O-2+C6H12OOH2-1O 9.000E+12 0.000 -1000.0 C6H12OOH2-3O2+C6H13-2=¿C6H13O-2+C6H12OOH2-3O 9.000E+12 0.000 -1000.0 C6H12OOH2-4O2+C6H13-2=¿C6H13O-2+C6H12OOH2-4O 9.000E+12 0.000 -1000.0 C6H12OOH2-5O2+C6H13-2=¿C6H13O-2+C6H12OOH2-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-6O2+C6H13-2=¿C6H13O-2+C6H12OOH2-6O 9.000E+12 0.000 -1000.0 C6H12OOH3-1O2+C6H13-2=¿C6H13O-2+C6H12OOH3-1O 9.000E+12 0.000 -1000.0 C6H12OOH3-2O2+C6H13-2=¿C6H13O-2+C6H12OOH3-2O 9.000E+12 0.000 -1000.0 C6H12OOH3-4O2+C6H13-2=¿C6H13O-2+C6H12OOH3-4O 9.000E+12 0.000 -1000.0 C6H12OOH3-5O2+C6H13-2=¿C6H13O-2+C6H12OOH3-5O 9.000E+12 0.000 -1000.0 C6H12OOH3-6O2+C6H13-2=¿C6H13O-2+C6H12OOH3-6O 9.000E+12 0.000 -1000.0 C6H12OOH1-2O2+C6H13-3=¿C6H13O-3+C6H12OOH1-2O 9.000E+12 0.000 -1000.0 C6H12OOH1-3O2+C6H13-3=¿C6H13O-3+C6H12OOH1-3O 9.000E+12 0.000 -1000.0 C6H12OOH1-4O2+C6H13-3=¿C6H13O-3+C6H12OOH1-

4O 9.000E+12 0.000 -1000.0 C6H12OOH1-5O2+C6H13-3=¿C6H13O-3+C6H12OOH1-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-1O2+C6H13-3=¿C6H13O-3+C6H12OOH2-1O 9.000E+12 0.000 -1000.0 C6H12OOH2-3O2+C6H13-3=¿C6H13O-3+C6H12OOH2-3O 9.000E+12 0.000 -1000.0 C6H12OOH2-4O2+C6H13-3=¿C6H13O-3+C6H12OOH2-4O 9.000E+12 0.000 -1000.0 C6H12OOH2-5O2+C6H13-3=¿C6H13O-3+C6H12OOH2-5O 9.000E+12 0.000 -1000.0 C6H12OOH2-6O2+C6H13-3=¿C6H13O-3+C6H12OOH2-6O 9.000E+12 0.000 -1000.0 C6H12OOH3-1O2+C6H13-3=¿C6H13O-3+C6H12OOH3-1O 9.000E+12 0.000 -1000.0 C6H12OOH3-2O2+C6H13-3=¿C6H13O-3+C6H12OOH3-2O 9.000E+12 0.000 -1000.0 C6H12OOH3-4O2+C6H13-3=¿C6H13O-3+C6H12OOH3-4O 9.000E+12 0.000 -1000.0 C6H12OOH3-5O2+C6H13-3=¿C6H13O-3+C6H12OOH3-5O 9.000E+12 0.000 -1000.0 C6H12OOH3-6O2+C6H13-3=¿C6H13O-3+C6H12OOH3-6O 9.000E+12 0.000 -1000.0 C5H8D14+OH=CH2O+C4H71-3 1.000E+12 0.000 0.0 C5H8D14+OH=C2H3CHO+C2H5 1.000E+12 0.000 0.0 C5H8D14+OH=CH3CHO+C3H5-S 1.000E+12 0.000 0.0 C6H12-1=C3H6+C3H6 4.000E+12 0.000 58000.0 C6H12-1=NC3H7+C3H5-A 8.000E+15 0.000 70000.0 C6H12-2=C2H5+C4H71-3 8.000E+15 0.000 70000.0 C6H12-3=CH3+C5H91-3 1.000E+16 0.000 73000.0 C6H111-3+H=C6H12-1 1.000E+14 0.000 0.0 C5H91-5+CH3=C6H12-1 1.000E+13 0.000 0.0 PC4H9+C2H3=C6H12-1 1.000E+13 0.000 0.0 C4H71-4+C2H5=C6H12-1 8.000E+12 0.000 0.0 C6H111-3+H=C6H12-2 1.000E+14 0.000 0.0 C6H112-4+H=C6H12-2 1.000E+14 0.000 0.0 C5H92-5+CH3=C6H12-2 1.000E+13 0.000 0.0 NC3H7+C3H5-T=C6H12-2 1.000E+13 0.000 0.0 C6H112-4+H=C6H12-3 1.000E+14 0.000 0.0 C4H71-1+C2H5=C6H12-3 1.000E+13 0.000 0.0 C6H12-1+OH=¿PC4H9+CH3CHO 1.000E+11 0.000 -2000.0 C6H12-2+OH=¿CH3+PC4H9CHO 5.000E+10 0.000 -2000.0 C6H12-2+OH=¿C2H5CHO+NC3H7 5.000E+10 0.000 -2000.0 C6H12-3+OH=¿PC4H9+CH3CHO 1.000E+11 0.000 -4000.0 C5H10-1+OH=NC3H7+CH3CHO 1.000E+11 0.000 -2000.0 C5H10-2+OH=CH3+NC3H7CHO 1.000E+11 0.000 -2000.0 C6H12-1+O=C5H11-1+HCO 1.000E+11 0.000 -1050.0 C6H12-2+O=PC4H9+CH3CO 1.000E+11 0.000 -1050.0 C6H12-1+H=C6H111-3+H2 3.380E+05 2.360 207.0 C6H12-1+O=C6H111-3+OH 6.600E+05 2.430 1210.0 C6H12-1+OH=C6H111-3+H2O 2.760E+04 2.640 -1919.0 C6H12-1+O2=C6H111-3+HO2 2.200E+12 0.000 37220.0 C6H12-1+HO2=C6H111-3+H2O2 4.820E+03 2.550 10530.0 C6H12-1+CH3=C6H111-3+CH4 3.690E+00 3.310 4002.0 C6H12-1+CH3O=C6H111-3+CH3OH 4.000E+01 2.900 8609.0 C6H12-1+CH3O2=C6H111-3+CH3O2H 4.820E+03 2.550 10530.0 C6H12-1+H=C6H111-4+H2 1.300E+06 2.400 4471.0 C6H12-1+O=C6H111-4+OH 2.810E+13 0.000 5200.0 C6H12-1+OH=C6H111-4+H2O 5.700E+06 1.811 -1016.0 C6H12-1+O2=C6H111-4+HO2 1.400E+13 0.000 50160.0 C6H12-1+HO2=C6H111-4+H2O2 9.480E+01 3.370 13720.0 C6H12-1+CH3=C6H111-4+CH4 1.510E+00 3.460 5481.0 C6H12-1+CH3O=C6H111-4+CH3OH 1.450E+11 0.000 4571.0 C6H12-1+CH3O2=C6H111-4+CH3O2H 1.020E+01 3.580 14810.0

C6H12-1+H=C6H111-5+H2 1.300E+06 2.400 4471.0 C6H12-1+O=C6H111-5+OH 2.810E+13 0.000 5200.0 C6H12-1+OH=C6H111-5+H2O 7.050E+09 0.935 505.0 C6H12-1+O2=C6H111-5+HO2

1.400E+13 0.000 50160.0 C6H12-1+HO2=C6H111-5+H2O2 9.480E+01 3.370 13720.0 C6H12-1+CH3=C6H111-5+CH4 1.510E+00 3.460 5481.0 C6H12-1+CH3O=C6H111-5+CH3OH 1.450E+11 0.000 4571.0 C6H12-1+CH3O2=C6H111-5+CH3O2H 1.020E+01 3.580 14810.0 C6H12-1+H=C6H111-6+H2 1.745E+05 2.690 6450.0 C6H12-1+O=C6H111-6+OH 5.650E+13 0.000 7850.0 C6H12-1+OH=C6H111-6+H2O 1.365E+07 1.813 868.0 C6H12-1+O2=C6H111-6+HO2 2.100E+13 0.000 52800.0 C6H12-1+HO2=C6H111-6+H2O2 2.040E+01 3.590 17160.0 C6H12-1+CH3=C6H111-6+CH4 4.520E-01 3.650 7154.0 C6H12-1+CH3O=C6H111-6+CH3OH 2.170E+11 0.000 6458.0 C6H12-1+CH3O2=C6H111-6+CH3O2H 6.950E-01 3.970 18280.0 C6H12-2+H=C6H111-3+H2 1.730E+05 2.500 2492.0 C6H12-2+O=C6H111-3+OH 4.410E+05 2.420 3150.0 C6H12-2+OH=C6H111-3+H2O 3.120E+06 2.000 -298.0 C6H12-2+O2=C6H111-3+HO2 3.300E+12 0.000 39900.0 C6H12-2+HO2=C6H111-3+H2O2 9.640E+03 2.600 13910.0 C6H12-2+CH3=C6H111-3+CH4 2.210E+00 3.500 5675.0 C6H12-2+CH3O=C6H111-3+CH3OH 9.000E+01 2.950 11990.0 C6H12-2+CH3O2=C6H111-3+CH3O2H 9.640E+03 2.600 13910.0 C6H12-2+H=C6H112-4+H2 3.380E+05 2.360 207.0 C6H12-2+O=C6H112-4+OH 6.600E+05 2.430 1210.0 C6H12-2+OH=C6H112-4+H2O 2.760E+04 2.640 -1919.0 C6H12-2+O2=C6H112-4+HO2 2.200E+12 0.000 37220.0 C6H12-2+HO2=C6H112-4+H2O2 4.820E+03 2.550 10530.0 C6H12-2+CH3=C6H112-4+CH4 3.690E+00 3.310 4002.0 C6H12-2+CH3O=C6H112-4+CH3OH 4.000E+01 2.900 8609.0 C6H12-2+CH3O2=C6H112-4+CH3O2H 4.820E+03 2.550 10530.0 C6H12-2+H=C6H112-5+H2 1.300E+06 2.400 4471.0 C6H12-2+O=C6H112-5+OH 2.810E+13 0.000 5200.0 C6H12-2+OH=C6H112-5+H2O 7.050E+09 0.935 505.0 C6H12-2+O2=C6H112-5+HO2 1.400E+13 0.000 50160.0 C6H12-2+HO2=C6H112-5+H2O2 9.480E+01 3.370 13720.0 C6H12-2+CH3=C6H112-5+CH4 1.510E+00 3.460 5481.0 C6H12-2+CH3O=C6H112-5+CH3OH 1.450E+11 0.000 4571.0 C6H12-2+CH3O2=C6H112-5+CH3O2H 1.020E+01 3.580 14810.0 C6H12-2+H=C6H112-6+H2 1.745E+05 2.690 6450.0 C6H12-2+O=C6H112-6+OH 5.650E+13 0.000 7850.0 C6H12-2+OH=C6H112-6+H2O 1.365E+07 1.813 868.0 C6H12-2+O2=C6H112-6+HO2 2.100E+13 0.000 52800.0 C6H12-2+HO2=C6H112-6+H2O2 2.040E+01 3.590 17160.0 C6H12-2+CH3=C6H112-6+CH4 4.520E-01 3.650 7154.0 C6H12-2+CH3O=C6H112-6+CH3OH 2.170E+11 0.000 6458.0 C6H12-2+CH3O2=C6H112-6+CH3O2H 6.950E-01 3.970 18280.0 C6H12-3+H=C6H113-1+H2 3.490E+05 2.690 6450.0 C6H12-3+O=C6H113-1+OH 1.130E+14 0.000 7850.0 C6H12-3+OH=C6H113-1+H2O 2.730E+07 1.813 868.0 C6H12-3+O2=C6H113-1+HO2 4.200E+13 0.000 52800.0 C6H12-3+HO2=C6H113-1+H2O2 4.080E+01 3.590 17160.0 C6H12-3+CH3=C6H113-1+CH4 9.040E-01 3.650 7154.0 C6H12-3+CH3O=C6H113-1+CH3OH 4.340E+11 0.000 6458.0 C6H12-3+CH3O2=C6H113-1+CH3O2H 1.390E+00 3.970 18280.0 C6H12-3+H=C6H112-4+H2 6.760E+05 2.360 207.0 C6H12-3+O=C6H112-4+OH 1.320E+06 2.430 1210.0 C6H12-3+OH=C6H112-4+H2O 5.520E+04 2.640 -1919.0 C6H12-3+O2=C6H112-4+HO2 4.400E+12 0.000 37220.0 C6H12-3+HO2=C6H112-4+H2O2 9.640E+03 2.550 10530.0 C6H12-3+CH3=C6H112-4+CH4 7.380E+00 3.310 4002.0 C6H12-3+CH3O=C6H112-4+CH3OH 8.000E+01 2.900 8609.0 C6H12-3+CH3O2=C6H112-4+CH3O2H 9.640E+03 2.550 10530.0

C6H12-1+O2CHO=C6H111-3+HO2CHO 4.820E+03 2.550 10530.0 C6H12-1+O2CHO=C6H111-4+HO2CHO 1.020E+01 3.580 14810.0 C6H12-1+O2CHO=C6H111-5+HO2CHO 1.020E+01 3.580 14810.0 C6H12-1+O2CHO=C6H111-6+HO2CHO 6.950E-01 3.970 18280.0 C6H12-2+O2CHO=C6H111-3+HO2CHO 9.640E+03 2.600 13910.0 C6H12-2+O2CHO=C6H112-4+HO2CHO 4.820E+03 2.550 10530.0 C6H12-2+O2CHO=C6H112-5+HO2CHO 1.020E+01 3.580 14810.0 C6H12-2+O2CHO=C6H112-6+HO2CHO 6.950E-01 3.970 18280.0 C6H12-3+O2CHO=C6H112-4+HO2CHO 9.640E+03 2.550 10530.0 C6H12-3+O2CHO=C6H113-1+HO2CHO 1.390E+00 3.970 18280.0 C6H111-6=C6H111-3 1.110E+12 0.000 31700.0 C6H12-1+H=C6H13-1 1.200E+09 1.300 1049.0 C6H12-1+H=C6H13-2 6.610E+08 1.400 -678.0 C6H12-2+H=C6H13-2 3.890E+08 1.600 580.0 C6H12-2+H=C6H13-3 3.890E+08 1.600 580.0 C6H12-3+H=C6H13-3 7.780E+08 1.600 580.0 C6H12-1+OH=C6H12OH-1J2 4.750E+12 0.000 0.0 C6H12-1+OH=C6H12OH-2J1 4.750E+12 0.000 0.0 C6H12-2+OH=C6H12OH-2J3 4.750E+12 0.000 0.0 C6H12-2+OH=C6H12OH-3J2 4.750E+12 0.000 0.0 C6H12-3+OH=C6H12OH-3J4 9.500E+12 0.000 0.0 C6H12OH-1J2+O2=C6H12OH-1O2-2 6.000E+12 0.000 0.0 C6H12OH-2J1+O2=C6H12OH-2O2-1 6.000E+12 0.000 0.0 C6H12OH-2J3+O2=C6H12OH-2O2-3 6.000E+12 0.000 0.0 C6H12OH-3J2+O2=C6H12OH-3O2-2 6.000E+12 0.000 0.0 C6H12OH-3J4+O2=C6H12OH-3O2-4 6.000E+12 0.000 0.0 C6H12OH-1O2-2=¿CH2O+PC4H9CHO+OH 2.000E+12 0.000 26800.0 C6H12OH-2O2-1=¿CH2O+PC4H9CHO+OH 2.000E+12 0.000 26800.0 C6H12OH-2O2-3=¿CH3CHO+NC3H7CHO 2.000E+12 0.000 26800.0 C6H12OH-3O2-2=¿CH3CHO+NC3H7CHO+OH 2.000E+12 0.000 26800.0 C6H12OH-3O2-4=¿C2H5CHO+C2H5CHO+OH 2.000E+12 0.000 26800.0 C6H111-3=C2H5+C4H6 1.000E+13 0.000 35000.0 CH3+C5H8D14=C6H111-4 1.000E+11 0.000 7800.0 C6H111-5=C3H5-A+C3H6 3.300E+13 0.00 22500.0 C6H111-6=C4H71-4+C2H4 2.000E+13 0.00 28700.0 CH3+C5H81-3=C6H112-4 1.000E+11 0.000 7800.0 C3H5-T+C3H6=C6H112-5 6.300E+11 0.000 3100.0 !C6H112-6=C4H72-1+C2H4 3.300E+13 0.00 22500.0 C4H71-1+C2H4=C6H113-1 6.300E+11 0.000 3100.0 C6H111-3+HO2=C6H11-1D3O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H111-3+CH3O2=C6H11-1D3O+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H111-3+C2H5O2=C6H11-1D3O+C2H5O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 /

PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H112-4+HO2=C6H11-2D4O+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H112-4+CH3O2=C6H11-2D4O+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H112-4+C2H5O2=C6H11-2D4O+C2H5O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / C6H111-3+HO2=C6H11-1D3OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01 1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06 0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13 -1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15 -1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17 -2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18 -2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19 -2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / C6H112-4+HO2=C6H11-2D4OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01 1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06 0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13 -1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15 -1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17 -2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18 -2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19 -2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / C6H111-3+O2=C6H10D13+HO2 1.070E+00 3.710 9322.0 C6H111-4+O2=C6H10D13+HO2 1.070E+00 3.710 7322.0 C6H111-4+O2=NC6D14+HO2 1.070E+00 3.710 9322.0 C6H111-5+O2=NC6D14+HO2 1.070E+00 3.710 9322.0 C6H111-5+O2=C6H101-5+HO2 1.070E+00 3.710 9322.0 C6H111-6+O2=C6H101-5+HO2 1.070E+00 3.710 9322.0 C6H112-4+O2=C6H10D13+HO2 1.070E+00 3.710 9322.0 C6H112-4+O2=C6H10D24+HO2 1.070E+00 3.710 9322.0 C6H112-5+O2=C6H10D24+HO2 1.070E+00 3.710 7322.0 C6H112-5+O2=NC6D14+HO2 1.070E+00 3.710 9322.0 C6H112-6+O2=NC6D14+HO2 1.070E+00 3.710 9322.0 C6H113-1+O2=C6H10D13+HO2 1.070E+00 3.710 7322.0 NC6D14+OH=C6H9-A+H2O 3.120E+06 2.000 -298.0 NC6D14+HO2=C6H9-A+H2O2 1.730E-01 4.000 12103.0 C6H11-1D3O=C2H3CHO+NC3H7 1.430E+20 -2.040 11230.0 C6H11-1D3O=NC3H7CHO+C2H3 2.400E+18 -1.630 23410.0 C6H11-2D4O=SC3H5CHO+C2H5 3.130E+19 -1.900 10670.0 NC5H11CHO+O2=NC5H11CO+HO2 3.010E+13 0.000 39150.0 NC5H11CHO+O=NC5 5.940E+12 0.000 1868.0 NC5H11CHO+H=NC5H11CO+H2 1.310E+05 2.580 1220.0 NC5H11CHO+OH=NC5H11 3.370E+12 0.000 -619.0 NC5H11CHO+HO2=NC5H11CO+H2O2 3.010E+12 0.000 11920.0 NC5H11CHO+CH3=N

7.080E-04 4.580 1966.0 NC5H11CHO+CH3O2=NC5H11CO+CH3O2H 3.010E+12 0.000 11920.0
NC5H11CHO+OH=NC5H10CHO-1+H2O 5.520E+02 3.120 -1176.0 NC5H11CHO+HO2=NC5H10CHO-
1+H2O2 3.440E+12 0.050 17880.0 NC5H11CHO+CH3O2=NC5H10CHO-1+CH3O2H 3.440E+12
0.050 17880.0 NC5H11CHO+OH=NC5H10CHO-2+H2O 4.680E+07 1.610 -35.0 NC5H11CHO+HO2=NC5H10CHO
2+H2O2 9.640E+03 2.600 13910.0 NC5H11CHO+CH3O2=NC5H10CHO-2+CH3O2H 9.640E+03
2.600 13910.0 NC5H11CHO+OH=NC5H10CHO-3+H2O 4.680E+07 1.610 -35.0 NC5H11CHO+HO2=NC5H10CHO
3+H2O2 9.640E+03 2.600 13910.0 NC5H11CHO+CH3O2=NC5H10CHO-3+CH3O2H 9.640E+03
2.600 13910.0 NC5H11CHO+OH=NC5H10CHO-4+H2O 4.680E+07 1.610 -35.0 NC5H11CHO+HO2=NC5H10CHO
4+H2O2 9.640E+03 2.600 13910.0 NC5H11CHO+CH3O2=NC5H10CHO-4+CH3O2H 9.640E+03
2.600 13910.0 NC5H11CHO+OH=NC5H10CHO-5+H2O 4.680E+07 1.610 -35.0 NC5H11CHO+HO2=NC5H10CHO
5+H2O2 9.640E+03 2.600 13910.0 NC5H11CHO+CH3O2=NC5H10CHO-5+CH3O2H 9.640E+03
2.600 13910.0 NC5H11CO=C5H11-1+CO 1.000E+11 0.000 9600.0 C2H3CHO+NC3H7=NC5H10CHO-
1 1.230E+11 0.000 7800.0 HCO+C5H10-1=NC5H10CHO-2 1.000E+11 0.000 6000.0 NC5H10CHO-
3=CH2CHO+C4H8-1 7.400E+11 0.000 21970.0 NC5H10CHO-4=CH2CH2CHO+C3H6 7.400E+11
0.000 21970.0 NC5H10CHO-5=C3H6CHO-1+C2H4 7.400E+11 0.000 21970.0 C6H111-3+O2=C6H112O2-
1 2.000E+12 0.000 0.0 C6H111-3+O2=C6H111O2-3 2.000E+12 0.000 0.0 C6H111-4+O2=C6H111O2-
4 7.540E+12 0.000 0.0 C6H111-5+O2=C6H111O2-5 7.540E+12 0.000 0.0 C6H111-6+O2=C6H111O2-
6 4.520E+12 0.000 0.0 C6H112-4+O2=C6H113O2-2 2.000E+12 0.000 0.0 C6H112-4+O2=C6H112O2-
4 2.000E+12 0.000 0.0 C6H112-5+O2=C6H112O2-5 7.540E+12 0.000 0.0 C6H112-6+O2=C6H112O2-
6 4.520E+12 0.000 0.0 C6H113-1+O2=C6H113O2-1 4.520E+12 0.000 0.0 C6H111O2-3=¿C6H10D13+HO2
1.000E+39 -8.110 40500.0 C6H111O2-4=¿C6H10D13+HO2 5.040E+38 -8.110 38500.0 C6H111O2-
5=¿C6H10D14+HO2 1.000E+39 -8.110 40500.0 C6H111O2-6=¿C6H101-5+HO2 1.000E+39 -8.110
40500.0 C6H111O2-5=¿C6H101-5+HO2 1.010E+43 -9.410 41500.0 C6H112O2-4=¿C6H10D24+HO2
1.000E+39 -8.110 40500.0 C6H112O2-5=¿C6H10D24+HO2 5.040E+38 -8.110 37500.0 C6H112O2-
6=¿C6H10D14+HO2 1.000E+39 -8.110 40500.0 C6H113O2-2=¿C6H10D13+HO2 1.010E+43 -
9.410 41500.0 C6H113O2-1=¿C6H10D13+HO2 5.040E+38 -8.110 37500.0 C6H111O2-3=C6H101OOH3-
4 2.000E+11 0.000 26450.0 C6H111O2-3=C6H101OOH3-5 2.500E+10 0.000 20450.0 C6H111O2-
3=C6H101OOH3-6 9.380E+09 0.000 21950.0 C6H111O2-4=C6H101OOH4-3 2.000E+11 0.000
24450.0 C6H111O2-4=C6H101OOH4-5 2.000E+11 0.000 26450.0 C6H111O2-4=C6H101OOH4-6
3.750E+10 0.000 24000.0 C6H111O2-5=C6H101OOH5-3 2.500E+10 0.000 18450.0 C6H111O2-
5=C6H101OOH5-4 2.000E+11 0.000 26450.0 C6H111O2-5=C6H101OOH5-6 3.000E+11 0.000
29000.0 C6H111O2-6=C6H101OOH6-3 3.120E+09 0.000 16650.0 C6H111O2-6=C6H101OOH6-4
2.500E+10 0.000 20450.0 C6H111O2-6=C6H101OOH6-5 2.000E+11 0.000 26450.0 C6H112O2-
4=C6H102OOH4-5 2.000E+11 0.000 26450.0 C6H112O2-4=C6H102OOH4-6 3.750E+10 0.000
24000.0 C6H112O2-5=C6H102OOH5-4 2.000E+11 0.000 24450.0 C6H112O2-5=C6H102OOH5-6
3.000E+11 0.000 29000.0 C6H112O2-6=C6H102OOH6-4 2.500E+10 0.000 18450.0 C6H112O2-

6=C6H102OOH6-5 2.000E+11 0.000 26450.0 C6H113O2-1=C6H103OOH1-2 2.000E+11 0.000
24450.0 C6H113O2-2=C6H103OOH2-1 3.000E+11 0.000 29000.0 C6H101OOH3-4=¿ETES1+OH
6.000E+11 0.000 22000.0 C6H101OOH3-5=¿MVOX+OH 7.500E+10 0.000 15250.0 C6H101OOH3-
4=¿VTHF+OH 9.380E+09 0.000 7000.0 C6H101OOH4-3=¿EDHF+OH 9.380E+09 0.000 7000.0
C6H101OOH4-3=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H101OOH4-5=¿ETES1+OH 6.000E+11
0.000 22000.0 C6H101OOH4-6=¿ETES1+OH 7.500E+10 0.000 15250.0 C6H101OOH5-3=¿MVOX+OH
7.500E+10 0.000 15250.0 C6H101OOH5-4=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H101OOH5-
6=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H101OOH6-3=¿VTHF+OH 9.380E+09 0.000 7000.0
C6H101OOH6-4=¿ETES1+OH 7.500E+10 0.000 15250.0 C6H101OOH6-5=¿ETES1+OH 6.000E+11
0.000 22000.0 C6H102OOH4-5=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H102OOH4-6=¿ETES1+OH
7.500E+10 0.000 15250.0 C6H102OOH5-4=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H102OOH5-
6=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H102OOH6-4=¿ETES1+OH 7.500E+10 0.000 15250.0
C6H102OOH6-5=¿ETES1+OH 6.000E+11 0.000 22000.0 C6H103OOH2-1=¿ETES1+OH 6.000E+11
0.000 22000.0 C6H103OOH1-2=¿ETES1+OH 6.000E+11 0.000 22000.0 HO2+C6H10D13=C6H101OOH3-
4 4.850E+11 0.000 10000.0 HO2+C6H10D13=C6H101OOH4-3 4.850E+11 0.000 9000.0 HO2+C6H10D14=C6H10
5 3.400E+11 0.000 11800.0 HO2+C6H10D14=C6H101OOH5-4 3.400E+11 0.000 11800.0 HO2+C6H101-
5=C6H101OOH5-6 1.000E+12 0.000 13700.0 HO2+C6H101-5=C6H101OOH6-5 1.000E+12 0.000
13700.0 HO2+C6H10D24=C6H102OOH4-5 3.800E+11 0.000 8800.0 HO2+C6H10D24=C6H102OOH5-
4 3.800E+11 0.000 7800.0 HO2+C6H10D14=C6H102OOH5-6 1.000E+12 0.000 13700.0 HO2+C6H10D14=C6H10
5 1.000E+12 0.000 13700.0 HO2+C6H10D13=C6H103OOH2-1 4.850E+11 0.000 10000.0 HO2+C6H10D13=C6H1
2 4.850E+11 0.000 9000.0 C6H101OOH3-4=¿CH3+AC3H5OOH+C2H2 3.000E+13 0.000 33500.0
C6H101OOH3-5=¿OH+C3H6+C2H3CHO 3.000E+13 0.000 23000.0 C6H101OOH3-6=¿HO2+C4H6+C2H4
3.000E+13 0.000 30000.0 C6H101OOH4-3=¿C2H5+CH3O2H+C3H2 1.000E+13 0.000 35000.0
C6H101OOH4-5=¿C3H5-A+AC3H5OOH 3.000E+13 0.000 23000.0 C6H101OOH4-6=¿OH+C2H3COCH3+C2H4
3.000E+13 0.000 30000.0 C6H101OOH5-3=¿OH+C4H6+CH3CHO 1.000E+13 0.000 35000.0 C6H101OOH5-
4=¿CH3+CH3O2H+2C2H2 3.000E+13 0.000 33500.0 C6H101OOH5-6=¿C4H71-4+C2H3OOH 3.000E+13
0.000 30000.0 C6H101OOH6-3=¿HO2+C4H6+C2H4 1.000E+13 0.000 35000.0 C6H101OOH6-
4=¿OH+C5H8D14+CH2O 3.000E+13 0.000 29500.0 C6H101OOH6-5=¿C3H5-A+AC3H5OOH 3.000E+13
0.000 23000.0 C6H102OOH4-6=¿OH+C2H3COCH3+C2H4 3.000E+13 0.000 22000.0 C6H102OOH5-
6=¿C4H71-3+CH2CHO+OH 3.000E+13 0.000 22000.0 C6H102OOH6-4=¿OH+C5H81-3+CH2O
1.000E+13 0.000 35000.0 C6H102OOH6-5=¿C3H5-T+AC3H5OOH 3.000E+13 0.000 39000.0

C6H10D13+H=C6H111-3 2.500E+11 0.500 2620.0 C6H10D13+H=C6H111-4 2.500E+11 0.500
2620.0 C6H10D13+H=C6H113-1 4.250E+11 0.500 1230.0 C6H10D13+H=C6H112-4 2.500E+11
0.500 2620.0 C6H10D14+H=C6H111-4 2.500E+11 0.500 2620.0 C6H10D14+H=C6H111-5 2.500E+11
0.500 2620.0 C6H10D14+H=C6H112-5 4.250E+11 0.500 1230.0 C6H10D14+H=C6H112-6 2.500E+11

0.500 2620.0 C6H101-5+H=C6H111-5 4.250E+11 0.500 1230.0 C6H101-5+H=C6H111-6 2.500E+11
0.500 2620.0 C6H10D13+O=¿C5H91-3+HCO 2.000E+11 0.000 -1050.0 C6H10D14+O=¿C5H92-
5+HCO 2.000E+11 0.000 -1050.0 C6H101-5+O=¿C5H91-5+HCO 2.000E+11 0.000 -1050.0 C6H10D13+OH=¿C5H
3+CH2O 1.000E+12 0.000 0.0 C6H10D14+OH=¿C5H92-5+CH2O 1.000E+12 0.000 0.0 C6H101-
5+OH=¿C5H91-5+CH2O 1.000E+12 0.000 0.0 C6H10D13+OH=¿C2H3+C4H6+H2O 2.760E+04
2.640 -1919.0 C6H10D14+OH=¿C2H3+C4H6+H2O 2.760E+04 2.640 -1919.0 C6H101-5+OH=¿C2H3+C4H6+H2
2.760E+04 2.640 -1919.0 C6H10D13+HO2=¿C2H3+C4H6+H2O2 4.820E+03 2.550 10530.0 C6H10D14+HO2=¿C
4.820E+03 2.550 10530.0 C6H101-5+HO2=¿C2H3+C4H6+H2O2 4.820E+03 2.550 10530.0 C6H10D13+H=¿C2H3
3.380E+05 2.360 207.0 C6H10D14+H=¿C2H3+C4H6+H2 3.380E+05 2.360 207.0 C6H101-5+H=¿C2H3+C4H6+H
3.380E+05 2.360 207.0 O2+ETES1=¿HO2+C2H3COCH3+C2H3 2.040E+07 2.000 40722.0 H+ETES1=¿H2+C2H
2.570E+07 2.000 3951.0 OH+ETES1=¿H2O+C2H3COCH3+C2H3 4.790E+06 2.000 -2260.0 O+ETES1=¿OH+C2
1.620E+07 2.000 2580.0 HO2+ETES1=¿H2O2+C2H3COCH3+C2H3 6.460E+05 2.000 11888.0
HCO+ETES1=¿CH2O+C2H3COCH3+C2H3 1.520E+06 2.000 12360.0 CH3+ETES1=¿CH4+C2H3COCH3+C2H3
4.680E+05 2.000 4871.0 C2H5+ETES1=¿C2H6+C2H3COCH3+C2H3 2.760E+05 2.000 7658.0
CH3O+ETES1=¿CH3OH+C2H3COCH3+C2H3 5.140E+05 2.000 1584.0 CH3O2+ETES1=¿CH3O2H+C2H3COCH
9.130E+05 2.000 12360.0 O2+MVOX=¿HO2+C2H3COCH3+C2H3 2.040E+07 2.000 40722.0 H+MVOX=¿H2+C2
2.570E+07 2.000 3951.0 OH+MVOX=¿H2O+C2H3COCH3+C2H3 4.790E+06 2.000 -2260.0 O+MVOX=¿OH+C2
1.620E+07 2.000 2580.0 HO2+MVOX=¿H2O2+C2H3COCH3+C2H3 6.460E+05 2.000 11888.0
HCO+MVOX=¿CH2O+C2H3COCH3+C2H3 1.520E+06 2.000 12360.0 CH3+MVOX=¿CH4+C2H3COCH3+C2H3
4.680E+05 2.000 4871.0 C2H5+MVOX=¿C2H6+C2H3COCH3+C2H3 2.760E+05 2.000 7658.0
CH3O2+MVOX=¿CH3O2H+C2H3COCH3+C2H3 9.130E+05 2.000 12360.0 C2H3+MVOX=¿C2H4+C2H3COCH3
8.140E+05 2.000 4871.0 CH3O+MVOX=¿CH3OH+C2H3COCH3+C2H3 5.140E+05 2.000 1584.0
O2+VTHF=¿HO2+C2H3COCH3+C2H3 2.040E+07 2.000 40722.0 H+VTHF=¿H2+C2H3COCH3+C2H3
2.570E+07 2.000 3951.0 OH+VTHF=¿H2O+C2H3COCH3+C2H3 4.790E+06 2.000 -2260.0 O+VTHF=¿OH+C2H
1.620E+07 2.000 2580.0

C3H5-A+C3H5-A=C6H101-5 1.000E+11 0.000 0.0 PLOG / 0.039 7.520E+64 -15.935 20230.0
/ PLOG / 0.078 1.725E+60 -14.490 18600.0 / PLOG / 0.156 2.620E+55 -12.995 16700.0 / C6H101-
5+H=C6H9-A+H2 6.752E+05 2.360 207.0 C6H101-5+O2=C6H9-A+HO2 9.760E+01 3.480 34800.0

C6H101-5+CH3=C6H9-A+CH4 7.380E+00 3.310 4002.0 C4H6+C2H3=C6H9-A 8.800E+05
2.500 6130.0 C6H101-5+H=¿C3H4-A+C3H5-A+H2 1.000E+12 0.000 0.0 C6H101-5+H=C3H5-
A+C3H6 1.000E+13 0.000 0.0 IC6-1+H=IC6 1.000E+14 0.000 0.0 IC6-2+H=IC6 1.000E+14
0.000 0.0 IC6-3+H=IC6 1.000E+14 0.000 0.0 IC6-4+H=IC6 1.000E+14 0.000 0.0 IC6-5+H=IC6
1.000E+14 0.000 0.0 C5H11-2+CH3=IC6 1.000E+13 0.000 0.0 NC3H7+IC3H7=IC6 8.000E+12
0.000 0.0 IC4H9+C2H5=IC6 8.000E+12 0.000 0.0 DC5H11+CH3=IC6 1.000E+13 0.000 0.0 IC6+H=IC6-
1+H2 3.490E+05 2.690 6450.0 IC6+H=IC6-2+H2 6.020E+05 2.400 2583.0 IC6+H=IC6-3+H2

1.300E+06 2.400 4471.0 IC6+H=IC6-4+H2 1.300E+06 2.400 4471.0 IC6+H=IC6-5+H2 1.745E+05 2.690 6450.0

IC6+CH3=IC6-1+CH4 9.040E-01 3.650 7154.0 IC6+CH3=IC6-2+CH4 6.010E-10 6.360 893.0 IC6+CH3=IC6-3+CH4 1.510E+00 3.460 5481.0 IC6+CH3=IC6-4+CH4 1.510E+00 3.460 5481.0 IC6+CH3=IC6-5+CH4 4.520E-01 3.650 7154.0

IC6+C2H5=IC6-1+C2H6 1.000E+11 0.000 13400.0 IC6+C2H5=IC6-2+C2H6 1.000E+11 0.000 7900.0 IC6+C2H5=IC6-3+C2H6 5.000E+10 0.000 10400.0 IC6+C2H5=IC6-4+C2H6 5.000E+10 0.000 10400.0 IC6+C2H5=IC6-5+C2H6 5.000E+10 0.000 13400.0 IC6+C2H3=IC6-1+C2H4 1.000E+12 0.000 18000.0 IC6+C2H3=IC6-2+C2H4 2.000E+11 0.000 14300.0 IC6+C2H3=IC6-3+C2H4 4.000E+11 0.000 16800.0 IC6+C2H3=IC6-4+C2H4 4.000E+11 0.000 16800.0 IC6+C2H3=IC6-5+C2H4 5.000E+11 0.000 18000.0

IC6-1=C3H6+NC3H7 3.749E+15 -0.610 29712.3 IC6-1=C5H10-1+CH3 1.234E+13 0.350 31078.2 IC6-2=IC4H8+C2H5 1.051E+13 0.120 27626.8 IC6-3=C5H10-2+CH3 5.288E+12 0.370 31129.4 IC6-3=CC5H10+CH3 2.164E+10 1.110 29899.6 IC6-4=C3H6+IC3H7 8.108E+14 -0.350 26953.8 IC6-5=IC4H9+C2H4 2.018E+14 -0.230 29727.3

IC6-1=IC6-4 2.000E+11 0.000 18100.0 IC6-1=IC6-5 3.000E+11 0.000 14100.0 IC6-2=IC6-5 3.000E+11 0.000 21100.0

IC6D1+H=IC6D1-1A+H2 1.730E+05 2.500 2492.0 IC6D1+H=IC6D1-3+H2 3.380E+05 2.360 207.0 IC6D1+H=IC6D1-4+H2 1.300E+06 2.400 4471.0 IC6D1+H=IC6D1-5+H2 1.745E+05 2.690 6450.0 IC6D2+H=IC6D1-3+H2 3.460E+05 2.500 2492.0 IC6D2+H=IC6D3-2+H2 3.380E+05 2.360 207.0 IC6D2+H=IC6D2-5+H2 1.745E+05 2.690 6450.0 IC6D3+H=IC6D3-1+H2 3.490E+05 2.690 6450.0 IC6D3+H=IC6D3-2+H2 2.650E+06 2.200 0.0 IC6D3+H=IC6D4-3+H2 1.730E+05 2.500 2492.0 IC6D4+H=IC6D4-1+H2 3.490E+05 2.690 6450.0 IC6D4+H=IC6D4-2+H2 6.020E+05 2.400 2583.0 IC6D4+H=IC6D4-3+H2 3.380E+05 2.360 207.0

IC6D1+CH3=IC6D1-1A+CH4 2.210E+00 3.500 5675.0 IC6D1+CH3=IC6D1-3+CH4 3.690E+00 3.310 4002.0 IC6D1+CH3=IC6D1-4+CH4 1.510E+00 3.460 5481.0 IC6D1+CH3=IC6D1-5+CH4 4.520E-01 3.650 7154.0 IC6D2+CH3=IC6D1-3+CH4 4.420E+00 3.500 5675.0 IC6D2+CH3=IC6D3-2+CH4 3.690E+00 3.310 4002.0 IC6D2+CH3=IC6D2-5+CH4 4.520E-01 3.650 7154.0 IC6D3+CH3=IC6D3-1+CH4 9.040E-01 3.650 7154.0 IC6D3+CH3=IC6D3-2+CH4 4.610E+00 3.100 2330.0 IC6D3+CH3=IC6D4-3+CH4 2.210E+00 3.500 5675.0 IC6D4+CH3=IC6D4-1+CH4 9.040E-01 3.650 7154.0 IC6D4+CH3=IC6D4-2+CH4 6.010E-10 6.360 893.0 IC6D4+CH3=IC6D4-3+CH4 3.690E+00 3.310 4002.0

IC6-1=IC6D1+H 5.000E+12 0.000 40000.0 IC6-2=IC6D1+H 5.000E+12 0.000 43600.0 IC6-2=IC6D2+H 5.000E+12 0.000 43600.0 IC6-3=IC6D2+H 5.000E+12 0.000 36000.0 IC6-3=IC6D3+H

5.000E+12 0.000 37900.0 IC6-4=IC6D3+H 5.000E+12 0.000 37900.0 IC6-4=IC6D4+H 2.000E+13 0.000 40400.0 IC6-5=IC6D4+H 1.290E+13 0.000 38600.0

IC6D1-1A=C3H4-A+NC3H7 1.280E+28 -4.430 72400.0 IC6D1-3=B13DE2M+CH3 7.170E+20 -2.490 52200.0 IC6D1-4=C3H6+C3H5-T 1.330E+22 -2.890 53700.0 IC6D1-5=IC4H7+C2H4 4.960E+23 -3.550 43600.0 IC6D2-5=IC4H7-I1+C2H4 2.010E+17 -1.320 43300.0 IC6D3-1=C5H81-3+CH3 2.460E+12 -0.040 24200.0 IC6D3-2=IC6D13+H 2.190E+16 -0.520 49100.0 IC6D4-1=C3H6+C3H5-A 1.230E+18 -1.480 17200.0 IC6D4-2=IC4H8+C2H3 8.220E+12 -0.260 37300.0 IC6D4-3=C5H81-3+CH3 1.500E+15 -0.480 37500.0

C3H4-A+C3H5-A=IC6D14-1 1.000E+11 0.000 7800.0

IC6D1-5=IC6D1-1A 4.170E+11 0.000 26400.0 IC6D1=IC4H7+C2H5 1.000E+16 0.000 71000.0 IC6D2=CC5H9-B+CH3 1.000E+16 0.000 71000.0 IC6D3=C5H92-4+CH3 1.000E+16 0.000 71000.0 IC6D4=C3H5-A+IC3H7 1.000E+16 0.000 71000.0

IC6D4-2=IC6D24+H 1.320E+05 2.280 33246.0 NC5D124+H=NC5D124-5R+H2 6.650E+05 2.530 12240.0 NC5D124+O=NC5D124-5R+OH 3.750E+06 1.900 3740.0 NC5D124+OH=NC5D124-5R+H2O 3.100E+06 2.000 3430.0 C2H2+C3H3=NC5D124-5R 3.160E+11 0.000 6000.0 I3C6-1+H=I3C6 1.000E+14 0.000 0.0 I3C6-2+H=I3C6 1.000E+14 0.000 0.0 I3C6-3+H=I3C6 1.000E+14 0.000 0.0 I3C6-4+H=I3C6 1.000E+14 0.000 0.0 AC5H11+CH3=I3C6 1.000E+13 0.000 0.0 SC4H9+C2H5=I3C6 8.000E+12 0.000 0.0 C5H11-3+CH3=I3C6 1.000E+13 0.000 0.0 I3C6+H=I3C6-1+H2 3.490E+05 2.690 6450.0 I3C6+H=I3C6-2+H2 2.600E+06 2.400 4471.0 I3C6+H=I3C6-3+H2 6.020E+05 2.400 2583.0 I3C6+H=I3C6-4+H2 1.745E+05 2.690 6450.0 I3C6+O=I3C6-1+OH 1.130E+14 0.000 7850.0 I3C6+O=I3C6-2+OH 5.620E+13 0.000 5200.0 I3C6+O=I3C6-3+OH 3.970E+05 2.401 1150.0 I3C6+O=I3C6-4+OH 5.650E+13 0.000 7850.0 I3C6+OH=I3C6-1+H2O 2.731E+07 1.813 868.4 I3C6+OH=I3C6-2+H2O 1.410E+10 0.935 504.7 I3C6+OH=I3C6-3+H2O 4.720E+10 0.576 -69.6 I3C6+OH=I3C6-4+H2O 1.675E+06 2.080 375.6

I3C6+CH3=I3C6-1+CH4 9.040E-01 3.650 7154.0 I3C6+CH3=I3C6-2+CH4 3.020E+00 3.460 5481.0 I3C6+CH3=I3C6-3+CH4 6.010E-10 6.360 893.0 I3C6+CH3=I3C6-4+CH4 4.520E-01 3.650 7154.0 I3C6+HO2=I3C6-1+H2O2 4.080E+01 3.590 17160.0 I3C6+HO2=I3C6-2+H2O2 1.896E+02 3.370 13720.0 I3C6+HO2=I3C6-3+H2O2 6.500E+02 3.010 12090.0 I3C6+HO2=I3C6-4+H2O2 2.040E+01 3.590 17160.0 I3C6+CH3O2=I3C6-1+CH3O2H 1.390E+00 3.970 18280.0 I3C6+CH3O2=I3C6-2+CH3O2H 2.040E+01 3.580 14810.0 I3C6+CH3O2=I3C6-3+CH3O2H 2.620E+02 3.120 11100.0 I3C6+CH3O2=I3C6-4+CH3O2H 6.950E-01 3.970 18280.0 I3C6+CH3O=I3C6-1+CH3OH 4.340E+11 0.000 6458.0 I3C6+CH3O=I3C6-2+CH3OH 2.900E+11 0.000 4571.0 I3C6+CH3O=I3C6-3+CH3OH 1.900E+10 0.000 2800.0 I3C6+CH3O=I3C6-4+CH3OH 2.170E+11 0.000 6458.0 I3C6+O2=I3C6-

1+HO2 4.200E+13 0.000 52800.0 I3C6+O2=I3C6-2+HO2 2.800E+13 0.000 50160.0 I3C6+O2=I3C6-3+HO2 7.000E+12 0.000 48000.0 I3C6+O2=I3C6-4+HO2 2.100E+13 0.000 52800.0 I3C6+C2H5=I3C6-1+C2H6 1.000E+11 0.000 13400.0 I3C6+C2H5=I3C6-2+C2H6 1.000E+11 0.000 10400.0 I3C6+C2H5=I3C6-3+C2H6 1.000E+11 0.000 7900.0 I3C6+C2H5=I3C6-4+C2H6 5.000E+10 0.000 13400.0 I3C6+C2H3=I3C6-1+C2H4 1.000E+12 0.000 18000.0 I3C6+C2H3=I3C6-2+C2H4 8.000E+11 0.000 16800.0 I3C6+C2H3=I3C6-3+C2H4 2.000E+11 0.000 14300.0 I3C6+C2H3=I3C6-4+C2H4 5.000E+11 0.000 18000.0

I3C6-1=C2H4+SC4H9 3.077E+15 -0.560 26537.3 I3C6-2=C5H10-2+CH3 5.795E+11 0.660 30319.3 I3C6-2=C4H8-2+C2H5 1.206E+13 0.030 28430.6 I3C6-3=AC5H10+CH3 1.049E+10 1.340 28930.0 I3C6-4=C4H8-1+C2H5 2.075E+14 -0.270 28931.9 I3C6-1+O2=I3C6D1+HO2 8.047E+00 3.320 12857.2 I3C6-2+O2=I3C6D1+HO2 2.645E+01 3.230 10591.8 I3C6-2+O2=I3C6D2+HO2 4.024E+00 3.320 10857.0 I3C6-3+O2=I3C6D2+HO2 1.609E+01 3.320 12857.2 I3C6-3+O2=I3C6D3+HO2 2.645E+01 3.230 10591.8 I3C6-4+O2=I3C6D3+HO2 4.024E+00 3.320 10857.0 I3C6-1=I3C6-4 3.000E+11 0.000 21100.0 I3C6-1=I3C6-2 2.000E+11 0.000 18100.0

I3C6D1+H=I3C6D1-3+H2 2.650E+06 2.200 0.0 I3C6D1+H=I3C6D1-4+H2 1.745E+05 2.690 6450.0 I3C6D1+H=I3C6D1-5+H2 1.300E+06 2.400 4471.0 I3C6D1+H=I3C6D1-6+H2 1.745E+05 2.690 6450.0 I3C6D2+H=I3C6D1-3+H2 1.730E+05 2.500 2492.0 I3C6D2+H=I3C6D3-2+H2 1.730E+05 2.500 2492.0 I3C6D2+H=I3C6D2-5+H2 3.380E+05 2.360 207.0 I3C6D2+H=I3C6D2-6+H2 1.745E+05 2.690 6450.0 I3C6D3+H=I3C6D3-1+H2 3.490E+05 2.690 6450.0 I3C6D3+H=I3C6D3-2+H2 6.760E+05 2.360 207.0

I3C6D1+CH3=I3C6D1-3+CH4 4.610E+00 3.100 2330.0 I3C6D1+CH3=I3C6D1-4+CH4 4.520E-01 3.650 7154.0 I3C6D1+CH3=I3C6D1-5+CH4 1.510E+00 3.460 5481.0 I3C6D1+CH3=I3C6D1-6+CH4 4.520E-01 3.650 7154.0 I3C6D2+CH3=I3C6D1-3+CH4 2.210E+00 3.500 5675.0 I3C6D2+CH3=I3C6D3-2+CH4 2.210E+00 3.500 5675.0 I3C6D2+CH3=I3C6D2-5+CH4 3.690E+00 3.310 4002.0 I3C6D2+CH3=I3C6D2-6+CH4 4.520E-01 3.650 7154.0 I3C6D3+CH3=I3C6D3-1+CH4 9.040E-01 3.650 7154.0 I3C6D3+CH3=I3C6D3-2+CH4 7.380E+00 3.310 4002.0

I3C6-1=I3C6D1+H 4.000E+12 0.000 38600.0 I3C6-2=I3C6D1+H 2.000E+13 0.000 40400.0 I3C6-2=I3C6D2+H 5.000E+13 0.000 39000.0 I3C6-3=I3C6D2+H 5.000E+12 0.000 42600.0 I3C6-3=I3C6D3+H 5.000E+12 0.000 43600.0 I3C6-4=I3C6D3+H 5.000E+12 0.000 36000.0

CH3+B13DE2M=I3C6D1-3 1.000E+11 0.000 7800.0 C2H5+C4H6=I3C6D1-4 1.000E+11 0.000 7800.0 CH3+C5H81-3=I3C6D1-5 1.000E+11 0.000 7800.0 I3C6D1-6=C2H4+C4H71-3 3.300E+13 0.00 2.250e+04 C4H72-2+C2H4=I3C6D2-6 1.000E+11 0.000 7800.0 C4H71-2+C2H4=I3C6D3-1 1.000E+11 0.000 7800.0

C4H612+C2H3=I3C6D13-5 1.000E+11 0.000 7800.0 C4H5-I+C2H4=I3C6D13-6 1.000E+11

0.000 7800.0 I3C6D15-3+O2=C2H3COCH3+CH2CHO 1.200E+36 -7.250 33600.0 C4H6+C2H3=I3C6D15-4 1.000E+11 0.000 7800.0 I3C6D1-3+HO2=I3C6D1-3O+OH 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D2-5+HO2=I3C6D2-5O+OH 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D3-2+HO2=I3C6D3-2O+OH 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D1-3+HO2=I3C6D1-3OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.030E+01 1.240 -22589.0 / PLOG / 1.00E-01 1.850E+06 0.080 -18331.0 / PLOG / 1.00E+00 1.010E+13 -1.450 -11709.0 / PLOG / 2.00E+00 7.450E+14 -1.870 -9604.0 / PLOG / 5.00E+00 9.250E+16 -2.310 -6991.0 / PLOG / 1.00E+01 1.440E+18 -2.550 -5260.0 / PLOG / 3.00E+01 1.730E+19 -2.710 -3140.0 / PLOG / 5.00E+01 2.670E+19 -2.700 -2438.0 / I3C6D2-5+HO2=I3C6D2-5OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01 1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06 0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13 -1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15 -1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17 -2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18 -2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19 -2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / I3C6D3-2+HO2=I3C6D3-2OOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 1.030E+01 1.240 -22589.0 / PLOG / 1.00E-01 1.850E+06 0.080 -18331.0 / PLOG / 1.00E+00 1.010E+13 -1.450 -11709.0 / PLOG / 2.00E+00 7.450E+14 -1.870 -9604.0 / PLOG / 5.00E+00 9.250E+16 -2.310 -6991.0 / PLOG / 1.00E+01 1.440E+18 -2.550 -5260.0 / PLOG / 3.00E+01 1.730E+19 -2.710 -3140.0 / PLOG / 5.00E+01 2.670E+19 -2.700 -2438.0 / I3C6D1-3+CH3O2=I3C6D1-3O+CH3O 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D2-5+CH3O2=I3C6D2-5O+CH3O 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D3-2+CH3O2=I3C6D3-2O+CH3O 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D1-3+C2H5O2=I3C6D1-3O+C2H5O 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D2-5+C2H5O2=I3C6D2-5O+C2H5O 1.000E+11

0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D3-2+C2H5O2=I3C6D3-2O+C2H5O 1.000E+11 0.000 0.0 PLOG / 0.0100 5.100E+12 -0.158 -1417.0 / PLOG / 0.1000 2.490E+14 -0.642 -349.1 / PLOG / 1.0000 3.890E+17 -1.520 2379.2 / PLOG / 10.0000 1.470E+15 -0.684 3615.3 / PLOG / 100.0000 8.200E+03 2.740 1144.4 / I3C6D1-3O=C2H5COCH3+C2H3 7.813E+13 -0.250 22330.0 I3C6D1-4O=C5H91-3+CH2O 4.470E+15 -1.130 4140.0 I3C6D1-5O=C4H71-3+CH3CHO 4.470E+15 -1.130 4140.0 CC5H9-A+CH2O=I3C6D1-6O 6.250E+10 0.000 11900.0 I3C6D2-5O=C4H72-2+CH3CHO 3.240E+22 -2.590 30000.0 I3C6D2-6O=AC5H9-C+CH2O 6.880E+14 -0.890 7260.0 I3C6D3-1O=AC5H9-A2+CH2O 6.880E+14 -0.890 7260.0 I3C6D3-2O=C4H71-2+CH3CHO 3.231E+22 -2.630 30310.0 I3C6D1=C4H71-3+C2H5 1.302E+21 -1.639 76140.0 I3C6D1=C5H91-3+CH3 1.302E+21 -1.639 76140.0 I3C6D2=AC5H9-C+CH3 1.900E+20 -1.582 75930.0 I3C6D3=AC5H9-A2+CH3 3.800E+20 -1.582 75930.0 I3C6-1+O2=I3C6-1O2 6.863E+16 -1.627 198.7 I3C6-2+O2=I3C6-2O2 3.486E+14 -0.816 -536.5 I3C6-3+O2=I3C6-3O2 9.752E+11 0.325 -417.3 I3C6-4+O2=I3C6-4O2 6.863E+16 -1.627 198.7 I3C6-1+HO2=I3C6-1O+OH 4.440E+42 -8.670 21071.0 I3C6-2+HO2=I3C6-2O+OH 4.440E+42 -8.670 21071.0 I3C6-3+HO2=I3C6-3O+OH 4.440E+42 -8.670 21071.0 I3C6-4+HO2=I3C6-4O+OH 4.440E+42 -8.670 21071.0 I3C6-1+CH3O2=I3C6-1O+CH3O 4.440E+42 -8.670 21071.0 I3C6-2+CH3O2=I3C6-2O+CH3O 4.440E+42 -8.670 21071.0 I3C6-3+CH3O2=I3C6-3O+CH3O 4.440E+42 -8.670 21071.0 I3C6-4+CH3O2=I3C6-4O+CH3O 4.440E+42 -8.670 21071.0 I3C6-1+I3C6-1O2=I3C6-1O+I3C6-1O 4.440E+42 -8.670 21071.0 I3C6-2+I3C6-1O2=I3C6-2O+I3C6-1O 4.440E+42 -8.670 21071.0 I3C6-3+I3C6-1O2=I3C6-3O+I3C6-1O 4.440E+42 -8.670 21071.0 I3C6-4+I3C6-1O2=I3C6-4O+I3C6-1O 4.440E+42 -8.670 21071.0 I3C6-1+I3C6-2O2=I3C6-1O+I3C6-2O 4.440E+42 -8.670 21071.0 I3C6-2+I3C6-2O2=I3C6-2O+I3C6-2O 4.440E+42 -8.670 21071.0 I3C6-3+I3C6-2O2=I3C6-3O+I3C6-2O 4.440E+42 -8.670 21071.0 I3C6-4+I3C6-2O2=I3C6-4O+I3C6-2O 4.440E+42 -8.670 21071.0 I3C6-1+I3C6-3O2=I3C6-1O+I3C6-3O 4.440E+42 -8.670 21071.0 I3C6-2+I3C6-3O2=I3C6-2O+I3C6-3O 4.440E+42 -8.670 21071.0 I3C6-3+I3C6-3O2=I3C6-3O+I3C6-3O 4.440E+42 -8.670 21071.0 I3C6-4+I3C6-3O2=I3C6-4O+I3C6-3O 4.440E+42 -8.670 21071.0 I3C6-1+I3C6-4O2=I3C6-1O+I3C6-4O 4.440E+42 -8.670 21071.0 I3C6-2+I3C6-4O2=I3C6-2O+I3C6-4O 4.440E+42 -8.670 21071.0 I3C6-3+I3C6-4O2=I3C6-3O+I3C6-4O 4.440E+42 -8.670 21071.0 I3C6-4+I3C6-4O2=I3C6-4O+I3C6-4O 4.440E+42 -8.670 21071.0 I3C6-1O2=I3C6OOH1-2 4.010E+08 1.100 30100.0 I3C6-1O2=I3C6OOH1-3 1.230E+07 1.200 15400.0 I3C6-1O2=I3C6OOH1-4 1.230E+06 1.500 20000.0 I3C6-1O2=I3C6OOH1-5 3.720E+06 1.200 16600.0 I3C6-1O2=I3C6OOH1-6 2.940E+05 1.500 19900.0 I3C6-2O2=I3C6OOH2-1 1.460E+09 1.100 33500.0 I3C6-2O2=I3C6OOH2-3 7.450E+09 0.600 27300.0 I3C6-2O2=I3C6OOH2-4 1.440E+07 1.400 20800.0 I3C6-2O2=I3C6OOH2-5 7.030E+10 0.200 18500.0 I3C6-2O2=I3C6OOH2-6 1.230E+06 1.500 20000.0 I3C6-3O2=I3C6OOH3-1 3.010E+08 1.100 21900.0 I3C6-3O2=I3C6OOH3-2 1.300E+10 0.700 30100.0 I3C6-3O2=I3C6OOH3-4 3.010E+09 1.200 33500.0

I3C6-4O2=I3C6OOH4-1 2.470E+06 1.500 20000.0 I3C6-4O2=I3C6OOH4-2 2.720E+07 1.300 18200.0
I3C6-4O2=I3C6OOH4-3 4.620E+09 0.800 27100.0 I3C6-1O2=I3C6D1+HO2 3.870E+07 1.580 28500.0
I3C6-2O2=I3C6D1+HO2 3.605E+09 1.130 30600.0 I3C6-2O2=I3C6D2+HO2 7.000E+10 0.710
30100.0 I3C6-3O2=I3C6D2+HO2 2.248E+11 0.580 29600.0 I3C6-3O2=I3C6D3+HO2 1.224E+10
0.890 29500.0 I3C6-4O2=I3C6D3+HO2 2.520E+08 1.320 27900.0 I3C6-1O2+HO2=I3C6-1OOH+O2
1.750E+10 0.000 -3275.0 I3C6-2O2+HO2=I3C6-2OOH+O2 1.750E+10 0.000 -3275.0 I3C6-3O2+HO2=I3C6-
3OOH+O2 1.750E+10 0.000 -3275.0 I3C6-4O2+HO2=I3C6-4OOH+O2 1.750E+10 0.000 -3275.0
I3C6-1O2+H2O2=I3C6-1OOH+HO2 2.400E+12 0.000 10000.0 I3C6-2O2+H2O2=I3C6-2OOH+HO2
2.400E+12 0.000 10000.0 I3C6-3O2+H2O2=I3C6-3OOH+HO2 2.400E+12 0.000 10000.0 I3C6-
4O2+H2O2=I3C6-4OOH+HO2 2.400E+12 0.000 10000.0 I3C6-1O2+I3C6=I3C6-1OOH+I3C6-1
1.210E+13 0.000 20430.0 I3C6-2O2+I3C6=I3C6-2OOH+I3C6-1 1.210E+13 0.000 20430.0 I3C6-
3O2+I3C6=I3C6-3OOH+I3C6-1 1.210E+13 0.000 20430.0 I3C6-4O2+I3C6=I3C6-4OOH+I3C6-1
1.210E+13 0.000 20430.0 I3C6-1O2+I3C6=I3C6-1OOH+I3C6-2 2.016E+12 0.000 16000.0 I3C6-
2O2+I3C6=I3C6-2OOH+I3C6-2 2.016E+12 0.000 16000.0 I3C6-3O2+I3C6=I3C6-3OOH+I3C6-2
2.016E+12 0.000 16000.0 I3C6-4O2+I3C6=I3C6-4OOH+I3C6-2 2.016E+12 0.000 16000.0 I3C6-
1O2+I3C6=I3C6-1OOH+I3C6-3 4.032E+12 0.000 17700.0 I3C6-2O2+I3C6=I3C6-2OOH+I3C6-3
4.032E+12 0.000 17700.0 I3C6-3O2+I3C6=I3C6-3OOH+I3C6-3 4.032E+12 0.000 17700.0 I3C6-
4O2+I3C6=I3C6-4OOH+I3C6-3 4.032E+12 0.000 17700.0 I3C6-1O2+I3C6=I3C6-1OOH+I3C6-4
6.048E+12 0.000 20430.0 I3C6-2O2+I3C6=I3C6-2OOH+I3C6-4 6.048E+12 0.000 20430.0 I3C6-
3O2+I3C6=I3C6-3OOH+I3C6-4 6.048E+12 0.000 20430.0 I3C6-4O2+I3C6=I3C6-4OOH+I3C6-4
6.048E+12 0.000 20430.0 I3C6-1O2+CH3O2=¿I3C6-1O+CH3O+O2 1.400E+16 -1.610 1860.0 I3C6-
2O2+CH3O2=¿I3C6-2O+CH3O+O2 1.400E+16 -1.610 1860.0 I3C6-3O2+CH3O2=¿I3C6-3O+CH3O+O2
1.400E+16 -1.610 1860.0 I3C6-4O2+CH3O2=¿I3C6-4O+CH3O+O2 1.400E+16 -1.610 1860.0 I3C6-
1O2+I3C6-1O2=¿I3C6-1O+I3C6-1O+O2 1.400E+16 -1.610 1860.0 I3C6-2O2+I3C6-1O2=¿I3C6-
2O+I3C6-1O+O2 1.400E+16 -1.610 1860.0 I3C6-3O2+I3C6-1O2=¿I3C6-3O+I3C6-1O+O2 1.400E+16
-1.610 1860.0 I3C6-4O2+I3C6-1O2=¿I3C6-4O+I3C6-1O+O2 1.400E+16 -1.610 1860.0 I3C6-2O2+I3C6-
2O2=¿I3C6-2O+I3C6-2O+O2 1.400E+16 -1.610 1860.0 I3C6-3O2+I3C6-2O2=¿I3C6-3O+I3C6-2O+O2
1.400E+16 -1.610 1860.0 I3C6-4O2+I3C6-2O2=¿I3C6-4O+I3C6-2O+O2 1.400E+16 -1.610 1860.0
I3C6-3O2+I3C6-3O2=¿I3C6-3O+I3C6-3O+O2 1.400E+16 -1.610 1860.0 I3C6-4O2+I3C6-3O2=¿I3C6-
4O+I3C6-3O+O2 1.400E+16 -1.610 1860.0 I3C6-4O2+I3C6-4O2=¿I3C6-4O+I3C6-4O+O2 1.400E+16
-1.610 1860.0 I3C6-1OOH=I3C6-1O+OH 1.500E+16 0.000 42000.0 I3C6-2OOH=I3C6-2O+OH
1.050E+16 0.000 41600.0 I3C6-3OOH=I3C6-3O+OH 6.000E+15 0.000 41200.0 I3C6-4OOH=I3C6-
4O+OH 1.500E+16 0.000 42000.0 CH2O+AC5H11=I3C6-1O 6.250E+10 0.000 11900.0 SC4H9CHO+CH3=I3C6-
2O 7.500E+10 0.000 11900.0 CH3CHO+SC4H9=I3C6-2O 7.500E+10 0.000 11900.0 C2H5COC2H5+CH3=I3C6-
3O 8.500E+10 0.000 11900.0 C2H5COCH3+C2H5=I3C6-3O 8.500E+10 0.000 11900.0 C5H11-
3+CH2O=I3C6-4O 6.250E+10 0.000 11900.0 I3C6OOH1-2=I3C6O1-2+OH 3.550E+12 0.000 8777.8

I3C6OOH1-3=I3C6O1-3+OH 1.268E+12 0.000 14704.3 I3C6OOH1-4=I3C6O1-4+OH 5.540E+10 0.000 8760.0 I3C6OOH1-5=I3C6O1-5+OH 2.770E+10 0.000 8676.9 I3C6OOH1-6=I3C6O1-6+OH 1.040E+10 0.000 10604.0 I3C6OOH2-1=I3C6O1-2+OH 3.550E+12 0.000 10435.7 I3C6OOH2-3=I3C6O2-3+OH 3.550E+12 0.000 8378.5 I3C6OOH2-4=I3C6O2-4+OH 6.340E+11 0.000 16118.1 I3C6OOH2-5=I3C6O2-5+OH 6.340E+11 0.000 16396.0 I3C6OOH2-6=I3C6O1-5+OH 2.770E+10 0.000 9748.6 I3C6OOH3-1=I3C6O1-3+OH 6.340E+11 0.000 17531.8 I3C6OOH3-2=I3C6O2-3+OH 3.550E+12 0.000 11016.5 I3C6OOH3-4=I3C6O3-4+OH 7.100E+12 0.000 11686.5 I3C6OOH4-1=I3C6O1-4+OH 5.540E+10 0.000 8760.0 I3C6OOH4-2=I3C6O2-4+OH 9.510E+11 0.000 15403.6 I3C6OOH4-3=I3C6O3-4+OH 3.550E+12 0.000 8390.6 I3C6OOH1-2=I3C6D1+HO2 6.240E+10 0.720 15000.0 I3C6OOH2-1=I3C6D1+HO2 1.780E+12 0.240 15700.0 I3C6OOH2-3=I3C6D2+HO2 7.820E+09 0.900 14900.0 I3C6OOH3-2=I3C6D2+HO2 3.010E+11 0.350 15200.0 I3C6OOH3-4=I3C6D3+HO2 3.890E+13 -0.150 15500.0 I3C6OOH4-3=I3C6D3+HO2 8.380E+09 0.920 14500.0 I3C6OOH1-3=¿AC5H10+CH2O+OH 3.081E+13 0.000 26297.1 I3C6OOH2-4=¿CH3CHO+C4H8-1+OH 3.081E+13 0.000 23542.0 I3C6OOH2-5=¿CH3CHO+C4H8-2+OH 3.081E+13 0.000 23738.1 I3C6OOH3-1=¿C2H5COCH3+C2H4+OH 3.081E+13 0.000 23216.3 I3C6OOH4-2=¿C5H10-2+CH2O+OH 3.081E+13 0.000 26196.4 I3C6OOH1-4=C4H8-1+C2H4O2H 1.392E+14 0.000 25690.5 I3C6OOH1-5=C4H8-2+C2H4O2H 1.392E+14 0.000 26034.6 I3C6OOH2-6=C2H4+C4H8OOH2-3 1.392E+14 0.000 26136.9 I3C6OOH4-1=C2H4+C4H8OOH1-2 1.392E+14 0.000 26136.9 I3C6OOH1-2+O2=I3C6OOH1-2O2 1.743E+14 -0.816 -536.5 I3C6OOH1-3+O2=I3C6OOH1-3O2 4.876E+11 0.325 -417.3 I3C6OOH1-4+O2=I3C6OOH1-4O2 3.431E+16 -1.627 198.7 I3C6OOH1-5+O2=I3C6OOH1-5O2 1.743E+14 -0.816 -536.5 I3C6OOH1-6+O2=I3C6OOH1-6O2 3.431E+16 -1.627 198.7 I3C6OOH2-1+O2=I3C6OOH2-1O2 3.431E+16 -1.627 198.7 I3C6OOH2-3+O2=I3C6OOH2-3O2 4.876E+11 0.325 -417.3 I3C6OOH2-4+O2=I3C6OOH2-4O2 3.431E+16 -1.627 198.7 I3C6OOH2-5+O2=I3C6OOH2-5O2 1.743E+14 -0.816 -536.5 I3C6OOH2-6+O2=I3C6OOH2-6O2 3.431E+16 -1.627 198.7 I3C6OOH3-1+O2=I3C6OOH3-1O2 3.431E+16 -1.627 198.7 I3C6OOH3-2+O2=I3C6OOH3-2O2 1.743E+14 -0.816 -536.5 I3C6OOH3-4+O2=I3C6OOH3-4O2 3.431E+16 -1.627 198.7 I3C6OOH4-1+O2=I3C6OOH4-1O2 3.431E+16 -1.627 198.7 I3C6OOH4-2+O2=I3C6OOH4-2O2 1.743E+14 -0.816 -536.5 I3C6OOH4-3+O2=I3C6OOH4-3O2 4.876E+11 0.325 -417.3 I3C6OOH1-2O2=I3C6KET1-2+OH 2.440E+07 1.600 27900.0 I3C6OOH1-3O2=I3C6KET1-3+OH 1.650E+04 2.400 19900.0 I3C6OOH1-4O2=I3C6KET1-4+OH 4.770E+03 1.700 16600.0 I3C6OOH1-5O2=I3C6KET1-5+OH 1.260E+03 2.200 17400.0 I3C6OOH1-6O2=I3C6KET1-6+OH 1.110E+03 1.800 16600.0 I3C6OOH2-1O2=I3C6KET2-1+OH 2.760E+08 1.200 25700.0 I3C6OOH2-3O2=I3C6KET2-3+OH 2.620E+08 1.700 26000.0 I3C6OOH2-4O2=I3C6KET2-4+OH 5.790E+01 2.900 17000.0 I3C6OOH2-5O2=I3C6KET2-5+OH 1.750E+02 3.100 17500.0 I3C6OOH2-6O2=I3C6KET2-6+OH 3.770E+02 2.200 15300.0 I3C6OOH4-1O2=I3C6KET4-1+OH 4.770E+03 1.700 16600.0 I3C6OOH4-2O2=I3C6KET4-2+OH 1.100E+04 2.400 19900.0 I3C6OOH4-3O2=I3C6KET4-3+OH 3.660E+07 1.600 27900.0 I3C6OOH3-1O2=I3C6D1-3OOH+HO2 3.870E+07 1.580 28500.0 I3C6OOH3-2O2=I3C6D1-3OOH+HO2

3.605E+09 1.130 30600.0 I3C6OOH4-1O2=I3C6D1-4OOH+HO2 3.870E+07 1.580 28500.0 I3C6OOH4-2O2=I3C6D1-4OOH+HO2 3.605E+09 1.130 30600.0 I3C6OOH2-5O2=I3C6D1-5OOH+HO2 3.605E+09 1.130 30600.0 I3C6OOH2-6O2=I3C6D1-5OOH+HO2 3.870E+07 1.580 28500.0 I3C6OOH1-5O2=I3C6D1-6OOH+HO2 3.605E+09 1.130 30600.0 I3C6OOH1-6O2=I3C6D1-6OOH+HO2 3.870E+07 1.580 28500.0 I3C6OOH1-2O2=I3C6D2-1OOH+HO2 7.000E+10 0.710 30100.0 I3C6OOH1-3O2=I3C6D2-1OOH+HO2 2.248E+11 0.580 29600.0 I3C6OOH4-2O2=I3C6D2-4OOH+HO2 7.000E+10 0.710 30100.0 I3C6OOH4-3O2=I3C6D2-4OOH+HO2 2.248E+11 0.580 29600.0 I3C6OOH2-3O2=I3C6D2-5OOH+HO2 1.124E+11 0.580 29600.0 I3C6OOH2-5O2=I3C6D2-5OOH+HO2 7.000E+10 0.710 30100.0 I3C6OOH1-3O2=I3C6D2-6OOH+HO2 2.248E+11 0.580 29600.0 I3C6OOH1-5O2=I3C6D2-6OOH+HO2 7.000E+10 0.710 30100.0 I3C6OOH1-3O2=I3C6D3-1OOH+HO2 1.224E+10 0.890 29500.0 I3C6OOH1-4O2=I3C6D3-1OOH+HO2 2.520E+08 1.320 27900.0 I3C6OOH2-3O2=I3C6D3-2OOH+HO2 1.224E+10 0.890 29500.0 I3C6OOH2-4O2=I3C6D3-2OOH+HO2 2.520E+08 1.320 27900.0 I3C6OOH1-2O2=I3C6Q12-3 7.450E+09 0.600 27300.0 I3C6OOH1-2O2=I3C6Q12-4 1.440E+07 1.400 20800.0 I3C6OOH1-2O2=I3C6Q12-5 7.030E+10 0.200 18500.0 I3C6OOH1-2O2=I3C6Q12-6 1.230E+06 1.500 20000.0 I3C6OOH1-3O2=I3C6Q13-2 6.510E+09 0.700 30100.0 I3C6OOH1-3O2=I3C6Q13-4 1.510E+09 1.200 33500.0 I3C6OOH1-3O2=I3C6Q13-5 6.510E+09 0.700 30100.0 I3C6OOH1-3O2=I3C6Q13-6 1.500E+08 1.100 21900.0 I3C6OOH1-4O2=I3C6Q14-2 1.360E+07 1.300 18200.0 I3C6OOH1-4O2=I3C6Q14-3 2.310E+09 0.800 27100.0 I3C6OOH1-4O2=I3C6Q14-5 1.360E+07 1.300 18200.0 I3C6OOH1-4O2=I3C6Q14-6 1.230E+06 1.500 20000.0 I3C6OOH1-5O2=I3C6Q15-2 7.030E+10 0.200 18500.0 I3C6OOH1-5O2=I3C6Q15-3 7.450E+09 0.600 27300.0 I3C6OOH1-5O2=I3C6Q15-4 1.440E+07 1.400 20800.0 I3C6OOH1-5O2=I3C6Q15-6 1.460E+09 1.100 33500.0 I3C6OOH1-6O2=I3C6Q16-2 3.720E+06 1.200 16600.0 DUP I3C6OOH1-6O2=I3C6Q16-3 1.230E+07 1.200 15400.0 I3C6OOH1-6O2=I3C6Q16-4 1.230E+06 1.500 20000.0 I3C6OOH1-6O2=I3C6Q16-2 4.010E+08 1.100 30100.0 DUP I3C6OOH2-1O2=I3C6Q12-3 1.230E+07 1.200 15400.0 I3C6OOH2-1O2=I3C6Q12-4 1.230E+06 1.500 20000.0 I3C6OOH2-1O2=I3C6Q12-5 3.720E+06 1.200 16600.0 I3C6OOH2-1O2=I3C6Q12-6 2.940E+05 1.500 19900.0 I3C6OOH2-3O2=I3C6Q23-1 1.500E+08 1.100 21900.0 I3C6OOH2-3O2=I3C6Q23-4 1.510E+09 1.200 33500.0 I3C6OOH2-3O2=I3C6Q23-5 6.510E+09 0.700 30100.0 I3C6OOH2-3O2=I3C6Q23-6 1.500E+08 1.100 21900.0 I3C6OOH2-4O2=I3C6Q24-1 1.230E+06 1.500 20000.0 I3C6OOH2-4O2=I3C6Q24-3 2.310E+09 0.800 27100.0 I3C6OOH2-4O2=I3C6Q24-5 1.360E+07 1.300 18200.0 I3C6OOH2-4O2=I3C6Q24-6 1.230E+06 1.500 20000.0 I3C6OOH2-5O2=I3C6Q25-1 1.230E+06 1.500 20000.0 DUP I3C6OOH2-5O2=I3C6Q25-3 7.450E+09 0.600 27300.0 I3C6OOH2-5O2=I3C6Q25-4 1.440E+07 1.400 20800.0 I3C6OOH2-5O2=I3C6Q25-1 1.460E+09 1.100 33500.0 DUP I3C6OOH2-6O2=I3C6Q15-6 2.940E+05 1.500 19900.0 I3C6OOH2-6O2=I3C6Q15-3 1.230E+07 1.200 15400.0 I3C6OOH2-6O2=I3C6Q15-4 1.230E+06 1.500 20000.0 I3C6OOH2-6O2=I3C6Q15-2 4.010E+08 1.100 30100.0 I3C6OOH3-1O2=I3C6Q13-2 4.010E+08 1.100 30100.0 I3C6OOH3-1O2=I3C6Q13-4 1.230E+06 1.500 20000.0 I3C6OOH3-1O2=I3C6Q13-5 3.720E+06

1.200 16600.0 I3C6OOH3-1O2=I3C6Q13-6 2.940E+05 1.500 19900.0 I3C6OOH3-2O2=I3C6Q23-1 1.460E+09 1.100 33500.0 I3C6OOH3-2O2=I3C6Q23-4 1.440E+07 1.400 20800.0 I3C6OOH3-2O2=I3C6Q23-5 7.030E+10 0.200 18500.0 I3C6OOH3-2O2=I3C6Q23-6 1.230E+06 1.500 20000.0 I3C6OOH3-4O2=I3C6Q34-1 2.470E+06 1.500 20000.0 I3C6OOH3-4O2=I3C6Q34-2 2.720E+07 1.300 18200.0 I3C6OOH4-1O2=I3C6Q14-2 4.010E+08 1.100 30100.0 I3C6OOH4-1O2=I3C6Q14-3 1.230E+07 1.200 15400.0 I3C6OOH4-1O2=I3C6Q14-5 3.720E+06 1.200 16600.0 I3C6OOH4-1O2=I3C6Q14-6 2.940E+05 1.500 19900.0 I3C6OOH4-2O2=I3C6Q24-1 1.460E+09 1.100 33500.0 I3C6OOH4-2O2=I3C6Q24-3 7.450E+09 0.600 27300.0 I3C6OOH4-2O2=I3C6Q24-5 7.030E+10 0.200 18500.0 I3C6OOH4-2O2=I3C6Q24-6 1.230E+06 1.500 20000.0 I3C6OOH4-3O2=I3C6Q34-1 3.010E+08 1.100 21900.0 I3C6OOH4-3O2=I3C6Q34-2 1.300E+10 0.700 30100.0 I3C6Q12-4=¿HO2CH2CHO+C4H8-1+OH 3.081E+13 0.000 25458.6 I3C6Q12-5=¿HO2CH2CHO+C4H8-2+OH 3.081E+13 0.000 25654.7 I3C6Q13-6=¿NC4KET24+C2H4+OH 3.081E+13 0.000 23433.7 I3C6Q14-5=¿C5H92-5OOH+CH2O+OH 3.081E+13 0.000 30622.4 I3C6Q15-4=¿C4H71-4OOH+CH3CHO+OH 3.081E+13 0.000 23542.0 I3C6Q16-3=¿C5H9A-DOOH+CH2O+OH 6.162E+13 0.000 26297.2 I3C6Q23-6=¿NC4KET23+C2H4+OH 3.081E+13 0.000 23433.7 I3C6Q24-5=¿C4H72-1OOH+CH3CHO+OH 3.081E+13 0.000 25497.9 I3C6Q24-5=¿C5H92-4OOH+CH2O+OH 3.081E+13 0.000 28035.7 I3C6Q25-4=¿C4H71-3OOH+CH3CHO+OH 6.162E+13 0.000 25360.1 I3C6Q34-1=¿NC4KET21+C2H4+OH 3.081E+13 0.000 25315.4 I3C6Q14-5=C4H72-1OOH+C2H4O2H 1.392E+14 0.000 36888.9 I3C6Q12-6=C4H72-3,4OOH+C2H4 1.392E+14 0.000 26136.9 I3C6Q14-6=C4H72-1,4OOH+C2H4 1.392E+14 0.000 33903.2 I3C6Q16-4=C4H71-4OOH+C2H4O2H 2.784E+14 0.000 25690.5 I3C6Q24-6=C4H72-1,3OOH+C2H4 1.392E+14 0.000 26136.9 I3C6KET1-2=I3C6KET1-2O+OH 1.050E+16 0.000 41800.0 I3C6KET1-3=I3C6KET1-3O+OH 6.000E+15 0.000 41300.0 I3C6KET1-4=I3C6KET1-4O+OH 1.500E+16 0.000 40800.0 I3C6KET1-5=I3C6KET1-5O+OH 1.050E+16 0.000 41800.0 I3C6KET1-6=I3C6KET1-6O+OH 1.500E+16 0.000 40800.0 I3C6KET2-1=I3C6KET2-1O+OH 1.500E+16 0.000 40800.0 I3C6KET2-3=I3C6KET2-3O+OH 6.000E+15 0.000 41300.0 I3C6KET2-4=I3C6KET2-4O+OH 1.500E+16 0.000 40800.0 I3C6KET2-5=I3C6KET2-5O+OH 1.050E+16 0.000 41800.0 I3C6KET2-6=I3C6KET2-6O+OH 1.500E+16 0.000 40800.0 I3C6KET4-1=I3C6KET4-1O+OH 1.500E+16 0.000 40800.0 I3C6KET4-2=I3C6KET4-2O+OH 1.050E+16 0.000 41800.0 I3C6KET4-3=I3C6KET4-3O+OH 1.200E+16 0.000 41300.0 I3C6KET1-2O=HCO+SC4H9CHO 2.900E+12 0.380 11080.0 I3C6KET1-3O=CH2CHO+C2H5COCH3 2.900E+12 0.380 11080.0 I3C6KET1-4O=PC4H8CHO-2+CH2O 2.900E+12 0.380 11080.0 I3C6KET1-5O=C3H6CHO-2+CH3CHO 2.900E+12 0.380 11080.0 I3C6KET1-6O=DC5H9O-A+CH2O 2.900E+12 0.380 11080.0 I3C6KET2-1O=SC4H9CO+CH2O 2.900E+12 0.380 11080.0 I3C6KET2-3O=CH3CO+C2H5COCH3 2.900E+12 0.380 11080.0 I3C6KET2-4O=CH3CH2CHCOCH3+CH2O 2.900E+12 0.380 11080.0 I3C6KET2-5O=CH3CHCOCH3+CH3CHO 2.900E+12 0.380 11080.0 I3C6KET2-6O=IC5Y3-1J+CH2O 2.900E+12 0.380 11080.0 I3C6KET4-1O=SC4H8CHO-1+CH2O 2.900E+12 0.380 11080.0 I3C6KET4-2O=C3H6CHO-3+CH3CHO 2.900E+12 0.380 11080.0 I3C6KET4-3O=HCO+C2H5COC2H5 5.800E+12

0.380 11080.0 I3C6Q12-3=I3C6D2-1OOH+HO2 7.820E+09 0.900 14900.0 I3C6Q13-2=I3C6D2-1OOH+HO2 3.010E+11 0.350 15200.0 I3C6Q13-2=I3C6D1-3OOH+HO2 6.240E+10 0.720 15000.0 I3C6Q13-4=I3C6D3-1OOH+HO2 3.890E+13 -0.150 15500.0 I3C6Q13-5=I3C6D2-6OOH+HO2 3.010E+11 0.350 15200.0 I3C6Q14-2=I3C6D1-4OOH+HO2 6.240E+10 0.720 15000.0 I3C6Q14-3=I3C6D3-1OOH+HO2 8.380E+09 0.920 14500.0 I3C6Q15-2=I3C6D1-5OOH+HO2 6.240E+10 0.720 15000.0 I3C6Q15-3=I3C6D2-6OOH+HO2 7.820E+09 0.900 14900.0 I3C6Q15-6=I3C6D1-6OOH+HO2 1.780E+12 0.240 15700.0 I3C6Q16-2=I3C6D1-6OOH+HO2 6.240E+10 0.720 15000.0 I3C6Q23-1=I3C6D1-3OOH+HO2 1.780E+12 0.240 15700.0 I3C6Q23-4=I3C6D3-2OOH+HO2 3.890E+13 -0.150 15500.0 I3C6Q23-5=I3C6D2-5OOH+HO2 3.010E+11 0.350 15200.0 I3C6Q24-1=I3C6D1-4OOH+HO2 1.780E+12 0.240 15700.0 I3C6Q24-3=I3C6D2-4OOH+HO2 7.820E+09 0.900 14900.0 I3C6Q24-3=I3C6D3-2OOH+HO2 8.380E+09 0.920 14500.0 I3C6Q25-1=I3C6D1-5OOH+HO2 1.780E+12 0.240 15700.0 I3C6Q25-3=I3C6D2-5OOH+HO2 7.820E+09 0.900 14900.0 I3C6Q34-2=I3C6D2-4OOH+HO2 3.010E+11 0.350 15200.0 I3C6D1-3OOH=¿C2H3COCH3+C2H5+OH 6.000E+15 0.000 41300.0 I3C6D1-3OOH=¿C2H3+C2H5 6.000E+15 0.000 41300.0 I3C6D3-1OOH=¿AC5H9-A2+CH2O+OH 1.500E+16 0.000 40800.0 I3C6D2-6OOH=¿AC5H9-C+CH2O+OH 1.500E+16 0.000 40800.0 I3C6D1-4OOH=¿C5H91-3+CH2O+OH 1.500E+16 0.000 40800.0 I3C6D1-5OOH=¿C4H71-3+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6D1-6OOH=¿CC5H9-A+CH2O+OH 1.500E+16 0.000 40800.0 I3C6D3-2OOH=¿C4H71-2+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6D2-5OOH=¿C4H72-2+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6Q12-3=I3C6O23-1OOH+OH 3.550E+12 0.000 8378.5 I3C6Q12-3=I3C6O13-2OOH+OH 1.268E+12 0.000 14871.5 I3C6Q12-4=I3C6O24-1OOH+OH 6.340E+11 0.000 16118.1 I3C6Q12-4=I3C6O14-2OOH+OH 5.540E+10 0.000 8760.0 I3C6Q12-5=I3C6O25-1OOH+OH 6.340E+11 0.000 16396.0 I3C6Q12-5=I3C6O15-2OOH+OH 2.770E+10 0.000 8676.9 I3C6Q12-6=I3C6O15-6OOH+OH 2.770E+10 0.000 9748.6 I3C6Q12-6=I3C6O16-2OOH+OH 1.040E+10 0.000 10604.0 I3C6Q13-2=I3C6O23-1OOH+OH 3.550E+12 0.000 11016.5 I3C6Q13-2=I3C6O12-3OOH+OH 3.550E+12 0.000 8777.8 I3C6Q13-4=I3C6O34-1OOH+OH 7.100E+12 0.000 11686.5 I3C6Q13-4=I3C6O14-3OOH+OH 5.540E+10 0.000 8817.0 I3C6Q13-5=I3C6O23-6OOH+OH 3.550E+12 0.000 11476.4 I3C6Q13-5=I3C6O15-3OOH+OH 2.770E+10 0.000 8676.9 I3C6Q13-6=I3C6O13-6OOH+OH 6.340E+11 0.000 17531.8 I3C6Q13-6=I3C6O16-3OOH+OH 1.040E+10 0.000 10604.0 I3C6Q14-2=I3C6O24-1OOH+OH 9.510E+11 0.000 21461.4 I3C6Q14-2=I3C6O12-4OOH+OH 3.550E+12 0.000 18882.3 I3C6Q14-3=I3C6O34-1OOH+OH 3.550E+12 0.000 18495.1 I3C6Q14-3=I3C6O13-4OOH+OH 1.268E+12 0.000 21218.2 I3C6Q14-5=I3C6O24-6OOH+OH 9.510E+11 0.000 21750.2 I3C6Q14-5=I3C6O15-4OOH+OH 2.770E+10 0.000 18196.8 I3C6Q14-6=I3C6O14-6OOH+OH 5.540E+10 0.000 18280.0 I3C6Q14-6=I3C6O16-4OOH+OH 1.040E+10 0.000 17451.7 I3C6Q15-2=I3C6O25-1OOH+OH 6.340E+11 0.000 16107.2 I3C6Q15-2=I3C6O12-5OOH+OH 3.550E+12 0.000 8777.8 I3C6Q15-3=I3C6O23-6OOH+OH 3.550E+12 0.000 8378.5 I3C6Q15-3=I3C6O13-5OOH+OH 1.268E+12 0.000 14871.5 I3C6Q15-4=I3C6O24-6OOH+OH 6.340E+11 0.000 16118.1 I3C6Q15-4=I3C6O14-5OOH+OH 5.540E+10 0.000 8760.0

I3C6Q15-6=I3C6O12-6OOH+OH 3.550E+12 0.000 10435.7 I3C6Q15-6=I3C6O16-2OOH+OH 1.040E+10 0.000 10645.0 I3C6Q16-2=I3C6O15-6OOH+OH 2.770E+10 0.000 8243.6 I3C6Q16-2=I3C6O12-6OOH+OH 3.550E+12 0.000 8777.8 I3C6Q16-3=I3C6O13-6OOH+OH 2.536E+12 0.000 14704.3 I3C6Q16-4=I3C6O14-6OOH+OH 1.108E+11 0.000 8760.0 I3C6Q23-1=I3C6O13-2OOH+OH 6.340E+11 0.000 17569.8 I3C6Q23-1=I3C6O12-3OOH+OH 3.550E+12 0.000 10435.7 I3C6Q23-4=I3C6O34-2OOH+OH 7.100E+12 0.000 11626.0 I3C6Q23-4=I3C6O24-3OOH+OH 6.340E+11 0.000 16118.1 I3C6Q23-5=I3C6O23-5OOH+OH 3.550E+12 0.000 11016.5 I3C6Q23-5=I3C6O25-3OOH+OH 6.340E+11 0.000 16107.2 I3C6Q23-6=I3C6O13-5OOH+OH 6.340E+11 0.000 17531.8 I3C6Q23-6=I3C6O15-3OOH+OH 2.770E+10 0.000 9748.6 I3C6Q24-1=I3C6O14-2OOH+OH 5.540E+10 0.000 8817.0 I3C6Q24-1=I3C6O12-4OOH+OH 3.550E+12 0.000 10435.7 I3C6Q24-3=I3C6O34-2OOH+OH 3.550E+12 0.000 8390.6 I3C6Q24-3=I3C6O23-4OOH+OH 3.550E+12 0.000 8378.5 I3C6Q24-5=I3C6O24-5OOH+OH 9.510E+11 0.000 15403.6 I3C6Q24-5=I3C6O25-4OOH+OH 6.340E+11 0.000 16396.0 I3C6Q24-6=I3C6O14-5OOH+OH 5.540E+10 0.000 8760.0 I3C6Q24-6=I3C6O15-4OOH+OH 2.770E+10 0.000 9748.6 I3C6Q25-1=I3C6O15-2OOH+OH 2.770E+10 0.000 9748.6 I3C6Q25-1=I3C6O12-5OOH+OH 3.550E+12 0.000 10375.2 I3C6Q25-3=I3C6O23-5OOH+OH 7.100E+12 0.000 8378.5 I3C6Q25-4=I3C6O24-5OOH+OH 1.268E+12 0.000 16118.1 I3C6Q34-1=I3C6O14-3OOH+OH 5.540E+10 0.000 8760.0 I3C6Q34-1=I3C6O13-4OOH+OH 6.340E+11 0.000 17531.8 I3C6Q34-2=I3C6O24-3OOH+OH 9.510E+11 0.000 15114.8 I3C6Q34-2=I3C6O23-4OOH+OH 3.550E+12 0.000 11016.5 I3C6O12-3OOH=¿CH2CHO+C2H5COCH3+OH 6.000E+15 0.000 41300.0 I3C6O12-4OOH=¿C5H9O2-1+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O12-5OOH=¿CH3CHO+C4H7O2-1+OH 1.050E+16 0.000 41800.0 I3C6O12-6OOH=¿IC5O34-1J+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O13-2OOH=¿C2H5COCH 1.050E+16 0.000 41800.0 I3C6O13-4OOH=¿CH2CH2COC2H5+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O13-5OOH=¿CH2CH2COCH3+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6O13-6OOH=¿AC5H9O-D+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O14-2OOH=¿C4H8-1+CH2OCHO+OH 1.050E+16 0.000 41800.0 I3C6O14-3OOH=¿CH2CH2COC2H5+CH2O+OH 6.000E+15 0.000 41300.0 I3C6O14-5OOH=¿C4H7O1-4+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6O14-6OOH=¿C4H71-4+2CH2O+OH 1.500E+16 0.000 40800.0 I3C6O15-2OOH=¿SC4H8CHO-3+CH2O+OH 1.050E+16 0.000 41800.0 I3C6O15-3OOH=¿CH2CH2COCH3+CH3CHO+OH 6.000E+15 0.000 41300.0 I3C6O15-4OOH=¿C5H9O2-5+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O15-6OOH=¿C4H8CHO4-2+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O16-2OOH=¿C4H8CHO4-2+CH2O+OH 1.050E+16 0.000 41800.0 I3C6O16-4OOH=¿C5H9O15-3+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O23-1OOH=¿SC4H8CHO-2+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O23-4OOH=¿CH3CHCOC2H5+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O23-5OOH=¿CH3CHCOCH3+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6O23-6OOH=¿AC5H9O-C+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O24-1OOH=¿SC4H8CHO-1+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O24-3OOH=¿CH3CHO+C2H5COCH2+OH 6.000E+15 0.000 41300.0 I3C6O24-5OOH=¿C4H7O2-1+CH3CHO+OH 1.050E+16 0.000 41800.0 I3C6O24-6OOH=¿C4H71-3+2CH2O+OH

1.500E+16 0.000 40800.0 I3C6O25-1OOH=¿SC4H8CHO-3+CH2O+OH 1.500E+16 0.000 40800.0
I3C6O25-3OOH=¿CH3CHCOCH3+CH3CHO+OH 1.200E+16 0.000 41300.0 I3C6O25-4OOH=¿C5H9O2-
4+CH2O+OH 1.500E+16 0.000 40800.0 I3C6O34-1OOH=¿AC5H9O-A2+CH2O+OH 1.500E+16
0.000 40800.0 I3C6O34-2OOH=¿CH3CHO+C2H5COCH2+OH 1.050E+16 0.000 41800.0 I3C6O1-
2+OH=¿SC3H5CHO+C2H5+H2O 2.500E+12 0.000 0.0 I3C6O1-2+OH=¿SC4H9+CH2CO+H2O
2.500E+12 0.000 0.0 I3C6O1-3+OH=¿AC5H10+HCO+H2O 2.500E+12 0.000 0.0 I3C6O1-4+OH=¿CH2CHO+C4H
1+H2O 2.500E+12 0.000 0.0 I3C6O1-4+OH=¿C2H4+C3H6CHO-3+H2O 2.500E+12 0.000 0.0
I3C6O1-5+OH=¿CH2CHO+C4H8-2+H2O 2.500E+12 0.000 0.0 I3C6O1-5+OH=¿CH3CHCOCH3+C2H4+H2O
2.500E+12 0.000 0.0 I3C6O1-6+OH=¿C2H4+C3H6CHO-2+H2O 5.000E+12 0.000 0.0 I3C6O2-
3+OH=¿IC3H5COCH3+CH3+H2O 2.500E+12 0.000 0.0 I3C6O2-4+OH=¿CH3CO+C4H8-1+H2O
2.500E+12 0.000 0.0 I3C6O2-4+OH=¿SC3H5CHO+C2H5+H2O 2.500E+12 0.000 0.0 I3C6O2-
5+OH=¿CH3CO+C4H8-2+H2O 5.000E+12 0.000 0.0 I3C6O1-2+HO2=¿SC3H5CHO+C2H5+H2O2
5.000E+12 0.000 17700.0 I3C6O1-2+HO2=¿SC4H9+CH2CO+H2O2 5.000E+12 0.000 17700.0
I3C6O1-3+HO2=¿AC5H10+HCO+H2O2 5.000E+12 0.000 17700.0 I3C6O1-4+HO2=¿CH2CHO+C4H8-
1+H2O2 5.000E+12 0.000 17700.0 I3C6O1-4+HO2=¿C2H4+C3H6CHO-3+H2O2 5.000E+12 0.000
17700.0 I3C6O1-5+HO2=¿CH2CHO+C4H8-2+H2O2 5.000E+12 0.000 17700.0 I3C6O1-5+HO2=¿CH3CHCOCH3
5.000E+12 0.000 17700.0 I3C6O1-6+HO2=¿C2H4+C3H6CHO-2+H2O2 5.000E+12 0.000 17700.0
I3C6O2-3+HO2=¿IC3H5COCH3+CH3+H2O2 5.000E+12 0.000 17700.0 I3C6O2-4+HO2=¿CH3CO+C4H8-
1+H2O2 5.000E+12 0.000 17700.0 I3C6O2-4+HO2=¿SC3H5CHO+C2H5+H2O2 5.000E+12 0.000
17700.0 I3C6O2-5+HO2=¿CH3CO+C4H8-2+H2O2 5.000E+12 0.000 17700.0 C3H6+CH2CHO=DC5H9O-
A 1.000E+11 0.000 7800.0 C5H9O2-1=C4H71-1+CH2O 4.320E+16 -1.000 29500.0 CH2O+C4H71-
4=C5H9O15-3 1.000E+11 0.000 7800.0 SC4H9CHO+O2=SC4H9CO+HO2 1.200E+05 2.500 37560.0
SC4H9CHO+OH=SC4H9CO+H2O 2.000E+06 1.800 -1300.0 SC4H9CHO+H=SC4H9CO+H2 4.140E+09
1.120 2320.0 SC4H9CHO+O=SC4H9CO+OH 5.940E+12 0.000 1868.0 SC4H9CHO+HO2=SC4H9CO+H2O2
4.090E+04 2.500 10200.0 SC4H9CHO+CH3=SC4H9CO+CH4 2.890E-03 4.620 3210.0 SC4H9CHO+CH3O=SC4H9
1.000E+12 0.000 3300.0 SC4H9CHO+CH3O2=SC4H9CO+CH3O2H 4.090E+04 2.500 10200.0
SC4H9CHO+OH=SC4H8CHO-1+H2O 5.280E+09 0.970 1586.0 SC4H9CHO+OH=SC4H8CHO-
2+H2O 5.520E+02 3.120 -1176.0 SC4H9CHO+OH=SC4H8CHO-3+H2O 4.680E+07 1.610 -35.0
SC4H9CHO+OH=C4H8CHO4-2+H2O 5.280E+09 0.970 1586.0 SC4H9CHO+HO2=SC4H8CHO-
1+H2O2 2.379E+04 2.550 16490.0 SC4H9CHO+HO2=SC4H8CHO-2+H2O2 3.440E+12 0.050
17880.0 SC4H9CHO+HO2=SC4H8CHO-3+H2O2 9.640E+03 2.600 13910.0 SC4H9CHO+HO2=C4H8CHO4-
2+H2O2 2.379E+04 2.550 16490.0 SC4H9CHO+CH3O2=SC4H8CHO-1+CH3O2H 2.379E+04 2.550
16490.0 SC4H9CHO+CH3O2=SC4H8CHO-2+CH3O2H 3.440E+12 0.050 17880.0 SC4H9CHO+CH3O2=SC4H8CH
3+CH3O2H 9.640E+03 2.600 13910.0 SC4H9CHO+CH3O2=C4H8CHO4-2+CH3O2H 2.379E+04
2.550 16490.0 SC4H9+HCO=SC4H9CHO 1.810E+13 0.000 0.0 SC4H9CO=SC4H9+CO 1.000E+11
0.000 9600.0 C2H3CHO+C2H5=SC4H8CHO-1 1.000E+11 0.000 6000.0 HCO+C4H8-1=SC4H8CHO-

1 1.000E+11 0.000 7800.0 CH3+IC3H5CHO=SC4H8CHO-2 1.000E+11 0.000 7800.0 HCO+C4H8-
2=SC4H8CHO-3 1.000E+11 0.000 6000.0 SC3H5CHO+CH3=SC4H8CHO-3 1.000E+11 0.000 7800.0
C2H5COC2H5+CH3O2=CH2CH2COC2H5+CH3O2H 2.379E+04 2.550 16490.0 C2H5COC2H5+CH3O2=CH3CHC
3.440E+12 0.050 17880.0 B13DE2M+O=B13DE2MJ+OH 1.050E+12 0.700 5884.0 NEC6-1+H=NEC6
1.000E+14 0.000 0.0 NEC6-3+H=NEC6 1.000E+14 0.000 0.0 NEC6-4+H=NEC6 1.000E+14 0.000
0.0 BC5H11+CH3=NEC6 1.000E+13 0.000 0.0 TC4H9+C2H5=NEC6 8.000E+12 0.000 0.0 NEOC5H11+CH3=NE
1.000E+13 0.000 0.0 NEC6+H=NEC6-1+H2 5.235E+05 2.690 6450.0 NEC6+H=NEC6-3+H2
1.300E+06 2.400 4471.0 NEC6+H=NEC6-4+H2 1.745E+05 2.690 6450.0 NEC6+O=NEC6-1+OH
1.695E+14 0.000 7850.0 NEC6+O=NEC6-3+OH 2.810E+13 0.000 5200.0 NEC6+O=NEC6-4+OH
5.650E+13 0.000 7850.0 NEC6+OH=NEC6-1+H2O 4.920E+07 1.760 743.0 NEC6+OH=NEC6-
3+H2O 5.720E+06 1.811 -1015.5 NEC6+OH=NEC6-4+H2O 1.365E+07 1.813 868.4 NEC6+CH3=NEC6-
1+CH4 1.356E+00 3.650 7154.0 NEC6+CH3=NEC6-3+CH4 1.510E+00 3.460 5481.0 NEC6+CH3=NEC6-
4+CH4 4.520E-01 3.650 7154.0 NEC6+HO2=NEC6-1+H2O2 6.120E+01 3.590 17160.0 NEC6+HO2=NEC6-
3+H2O2 9.480E+01 3.370 13720.0 NEC6+HO2=NEC6-4+H2O2 2.040E+01 3.590 17160.0 NEC6+CH3O2=NEC6-
1+CH3O2H 2.085E+00 3.970 18280.0 NEC6+CH3O2=NEC6-3+CH3O2H 1.020E+01 3.580 14810.0
NEC6+CH3O2=NEC6-4+CH3O2H 6.950E-01 3.970 18280.0 NEC6+CH3O=NEC6-1+CH3OH 6.510E+11
0.000 6458.0 NEC6+CH3O=NEC6-3+CH3OH 1.450E+11 0.000 4571.0 NEC6+CH3O=NEC6-4+CH3OH
2.170E+11 0.000 6458.0 NEC6+O2=NEC6-1+HO2 6.300E+13 0.000 52800.0 NEC6+O2=NEC6-
3+HO2 1.400E+13 0.000 50160.0 NEC6+O2=NEC6-4+HO2 2.100E+13 0.000 52800.0 NEC6+C2H5=NEC6-
1+C2H6 1.500E+11 0.000 13400.0 NEC6+C2H5=NEC6-3+C2H6 5.000E+10 0.000 10400.0 NEC6+C2H5=NEC6-
4+C2H6 5.000E+10 0.000 13400.0 NEC6+C2H3=NEC6-1+C2H4 1.500E+12 0.000 18000.0 NEC6+C2H3=NEC6-
3+C2H4 4.000E+11 0.000 16800.0 NEC6+C2H3=NEC6-4+C2H4 5.000E+11 0.000 18000.0 NEC6+O2CHO=NEC6
1+HO2CHO 2.085E+00 3.970 18280.0 NEC6+O2CHO=NEC6-3+HO2CHO 1.020E+01 3.580 14810.0
NEC6+O2CHO=NEC6-4+HO2CHO 6.950E-01 3.970 18280.0 NEC6-1=IC4H8+C2H5 1.926E+17 -
1.250 29506.3 NEC6-1=AC5H10+CH3 1.750E+15 -0.310 31619.5 NEC6-3=BC5H10+CH3 1.896E+16
-0.560 32723.5 NEC6-4=TC4H9+C2H4 1.100E+20 -1.870 25428.7 NEC6-3+O2=NEC6D3+HO2
2.645E+01 3.230 10591.8 NEC6-4+O2=NEC6D3+HO2 8.047E+00 3.320 12857.2 NEC6D3+OH=NEC6D3-
1+H2O 4.920E+07 1.760 743.0 NEC6D3+O=NEC6D3-1+OH 1.695E+14 0.000 7850.0 NEC6D3+H=NEC6D3-
1+H2 5.235E+05 2.690 6450.0 NEC6D3+CH3=NEC6D3-1+CH4 1.356E+00 3.650 7154.0 NEC6D3+HO2=NEC6D
1+H2O2 6.120E+01 3.590 17160.0 NEC6D3+CH3O=NEC6D3-1+CH3OH 6.510E+11 0.000 6458.0
NEC6D3+CH3O2=NEC6D3-1+CH3O2H 2.085E+00 3.970 18280.0 NEC6D3+O2=NEC6D3-1+HO2
6.300E+13 0.000 52800.0 NEC6D3+O2CHO=NEC6D3-1+HO2CHO 2.085E+00 3.970 18280.0 NEC6-
3=NEC6D3+H 2.000E+13 0.000 40400.0 NEC6-4=NEC6D3+H 1.290E+13 0.000 38600.0 NEC6D3+OH=CH3+TC
2.000E+10 0.000 4000.0 NEC6D3+OH=NEOC5H11+CH2O 2.000E+10 0.000 4000.0 NEC6D3+OH=NEC6OH3-
4J 1.000E+12 0.000 -1042.0 NEC6D3+OH=NEC6OH4-3J 1.000E+12 0.000 -1042.0 NEC6OH3-
4J+O2=NEC6OH3-4O2 2.000E+12 0.000 0.0 NEC6OH4-3J+O2=NEC6OH4-3O2 2.000E+12 0.000

0.0 NEC6OH3-4O2=¿TC4H9CHO+CH2O+OH 2.500E+10 0.000 18860.0 NEC6OH4-3O2=¿TC4H9CHO+CH2O+
2.500E+10 0.000 18860.0 NEC6D3-1=CH3+B13DE2M 4.792E+17 -1.230 29640.0 NEC6D3-1=C2H3+IC4H8
2.500E+13 0.000 45000.0 NEC6D3=CC5H9-B+CH3 1.000E+16 0.000 71000.0 NEC6-1+O2=NEC6-
1O2 6.863E+16 -1.627 198.7 NEC6-3+O2=NEC6-3O2 3.486E+14 -0.816 -536.5 NEC6-4+O2=NEC6-
4O2 9.752E+11 0.325 -417.3 NEC6-1+HO2=NEC6-1O+OH 4.440E+42 -8.670 21071.0 NEC6-
3+HO2=NEC6-3O+OH 4.440E+42 -8.670 21071.0 NEC6-4+HO2=NEC6-4O+OH 4.440E+42 -
8.670 21071.0 NEC6-1+CH3O2=NEC6-1O+CH3O 4.440E+42 -8.670 21071.0 NEC6-3+CH3O2=NEC6-
3O+CH3O 4.440E+42 -8.670 21071.0 NEC6-4+CH3O2=NEC6-4O+CH3O 4.440E+42 -8.670 21071.0
NEC6-1+NEC6-1O2=NEC6-1O+NEC6-1O 4.440E+42 -8.670 21071.0 NEC6-3+NEC6-1O2=NEC6-
3O+NEC6-1O 4.440E+42 -8.670 21071.0 NEC6-4+NEC6-1O2=NEC6-4O+NEC6-1O 4.440E+42 -
8.670 21071.0 NEC6-1+NEC6-3O2=NEC6-1O+NEC6-3O 4.440E+42 -8.670 21071.0 NEC6-3+NEC6-
3O2=NEC6-3O+NEC6-3O 4.440E+42 -8.670 21071.0 NEC6-4+NEC6-3O2=NEC6-4O+I3C6-3O
4.440E+42 -8.670 21071.0 NEC6-1+NEC6-4O2=NEC6-1O+NEC6-4O 4.440E+42 -8.670 21071.0
NEC6-3+NEC6-4O2=NEC6-3O+NEC6-4O 4.440E+42 -8.670 21071.0 NEC6-4+NEC6-4O2=NEC6-
4O+NEC6-4O 4.440E+42 -8.670 21071.0 NEC6-1O2=NEC6OOH1-1A 7.130E+06 1.600 21000.0
NEC6-1O2=NEC6OOH1-3 1.360E+07 1.300 18200.0 NEC6-1O2=NEC6OOH1-4 1.230E+06 1.500
20000.0 NEC6-3O2=NEC6OOH3-1 4.320E+07 1.400 20800.0 NEC6-3O2=NEC6OOH3-4 1.460E+09
1.100 33500.0 NEC6-4O2=NEC6OOH4-1 3.700E+06 1.500 20000.0 NEC6-4O2=NEC6OOH4-3 4.010E+08
1.100 30100.0 NEC6-3O2=NEC6D3+HO2 3.605E+09 1.130 30600.0 NEC6-4O2=NEC6D3+HO2
3.870E+07 1.580 28500.0 NEC6-1O2+HO2=NEC6-1OOH+O2 1.750E+10 0.000 -3275.0 NEC6-
3O2+HO2=NEC6-3OOH+O2 1.750E+10 0.000 -3275.0 NEC6-4O2+HO2=NEC6-4OOH+O2 1.750E+10
0.000 -3275.0 NEC6-1O2+H2O2=NEC6-1OOH+HO2 2.400E+12 0.000 10000.0 NEC6-3O2+H2O2=NEC6-
3OOH+HO2 2.400E+12 0.000 10000.0 NEC6-4O2+H2O2=NEC6-4OOH+HO2 2.400E+12 0.000
10000.0 NEC6-1O2+NEC6=NEC6-1OOH+NEC6-1 1.814E+13 0.000 20430.0 NEC6-3O2+NEC6=NEC6-
3OOH+NEC6-1 1.814E+13 0.000 20430.0 NEC6-4O2+NEC6=NEC6-4OOH+NEC6-1 1.814E+13
0.000 20430.0 NEC6-1O2+NEC6=NEC6-1OOH+NEC6-3 4.032E+12 0.000 17700.0 NEC6-3O2+NEC6=NEC6-
3OOH+NEC6-3 4.032E+12 0.000 17700.0 NEC6-4O2+NEC6=NEC6-4OOH+NEC6-3 4.032E+12
0.000 17700.0 NEC6-1O2+NEC6=NEC6-1OOH+NEC6-4 6.048E+12 0.000 20430.0 NEC6-3O2+NEC6=NEC6-
3OOH+NEC6-4 6.048E+12 0.000 20430.0 NEC6-4O2+NEC6=NEC6-4OOH+NEC6-4 6.048E+12
0.000 20430.0 NEC6-1O2+CH3O2=¿NEC6-1O+CH3O+O2 1.400E+16 -1.610 1860.0 NEC6-3O2+CH3O2=¿NEC6-
3O+CH3O+O2 1.400E+16 -1.610 1860.0 NEC6-4O2+CH3O2=¿NEC6-4O+CH3O+O2 1.400E+16
-1.610 1860.0 NEC6-1O2+NEC6-1O2=¿NEC6-1O+NEC6-1O+O2 1.400E+16 -1.610 1860.0 NEC6-
3O2+NEC6-1O2=¿NEC6-3O+NEC6-1O+O2 1.400E+16 -1.610 1860.0 NEC6-4O2+NEC6-1O2=¿NEC6-
4O+NEC6-1O+O2 1.400E+16 -1.610 1860.0 NEC6-3O2+NEC6-3O2=¿NEC6-3O+NEC6-3O+O2
1.400E+16 -1.610 1860.0 NEC6-4O2+NEC6-3O2=¿NEC6-4O+NEC6-3O+O2 1.400E+16 -1.610
1860.0 NEC6-4O2+NEC6-4O2=¿NEC6-4O+NEC6-4O+O2 1.400E+16 -1.610 1860.0 NEC6-1OOH=NEC6-

1O+OH 1.500E+16 0.000 41600.0 NEC6-3OOH=NEC6-3O+OH 1.050E+16 0.000 41200.0 NEC6-4OOH=NEC6-4O+OH 1.500E+16 0.000 41600.0 NEC6-1O=CH2O+BC5H11 5.500E+13 -0.210 18000.0 NEC6-3O=TC4H9CHO+CH3 1.280E+22 -2.580 21800.0 NEC6-3O=TC4H9+CH3CHO 7.270E+18 -1.460 19500.0 NEC6-4O=NEOC5H11+CH2O 1.830E+17 -1.280 20900.0 NEC6OOH1-1A=NEC6O1-1A+OH 6.340E+11 0.000 16125.7 NEC6OOH1-3=NEC6O1-3+OH 9.510E+11 0.000 15403.6 NEC6OOH1-4=NEC6O1-4+OH 5.540E+10 0.000 8760.0 NEC6OOH3-1=NEC6O1-3+OH 6.340E+11 0.000 16118.1 NEC6OOH3-4=NEC6O3-4+OH 3.550E+12 0.000 10435.7 NEC6OOH4-1=NEC6O1-4+OH 5.540E+10 0.000 8760.0 NEC6OOH4-3=NEC6O3-4+OH 3.550E+12 0.000 8777.8 NEC6OOH3-4=NEC6D3+HO2 1.780E+12 0.240 15700.0 NEC6OOH4-3=NEC6D3+HO2 6.240E+10 0.720 15000.0 NEC6OOH1-1A=¿AC5H10+CH2O+OH 3.081E+13 0.000 25337.8 NEC6OOH1-3=¿BC5H10+CH2O 3.081E+13 0.000 25555.1 NEC6OOH3-1=¿IC4H8+CH3CHO+OH 3.081E+13 0.000 22879.4 NEC6OOH1-4=IC4H8O2H-T+C2H4 1.392E+14 0.000 24230.1 NEC6OOH4-1=IC4H8+C2H4O2H 1.392E+14 0.000 24527.9 NEC6OOH1-1A+O2=NEC6OOH1-1AO2 3.430E+16 -1.627 198.7 NEC6OOH1-3+O2=NEC6OOH1-3O2 1.740E+14 -0.816 -536.5 NEC6OOH1-4+O2=NEC6OOH1-4O2 3.430E+16 -1.627 198.7 NEC6OOH3-1+O2=NEC6OOH3-1O2 3.430E+16 -1.627 198.7 NEC6OOH3-4+O2=NEC6OOH3-4O2 3.430E+16 -1.627 198.7 NEC6OOH4-1+O2=NEC6OOH4-1O2 3.430E+16 -1.627 198.7 NEC6OOH4-3+O2=NEC6OOH4-3O2 1.740E+14 -0.816 -536.5 NEC6OOH1-1AO2=NEC6KET1-1A+OH 5.190E+04 1.900 18800.0 NEC6OOH1-3O2=NEC6KET1-3+OH 1.100E+04 2.400 19900.0 NEC6OOH1-4O2=NEC6KET1-4+OH 4.770E+03 1.700 16600.0 NEC6OOH3-1O2=NEC6KET3-1+OH 5.790E+01 2.900 17000.0 NEC6OOH3-4O2=NEC6KET3-4+OH 2.760E+08 1.200 25700.0 NEC6OOH4-1O2=NEC6KET4-1+OH 4.770E+03 1.700 16600.0 NEC6OOH4-3O2=NEC6KET4-3+OH 2.440E+07 1.600 27900.0 NEC6OOH1-3O2=NEC6D3-1OOH+HO2 3.605E+09 1.130 30600.0 NEC6OOH1-4O2=NEC6D3-1OOH+HO2 3.870E+07 1.580 28500.0 NEC6OOH1-1AO2=NEC6Q11A-1B 3.570E+06 1.600 21000.0 NEC6OOH1-1AO2=NEC6Q11A-3 1.360E+07 1.300 18200.0 NEC6OOH1-1AO2=NEC6Q11A-4 1.230E+06 1.500 20000.0 NEC6OOH1-3O2=NEC6Q13-1A 2.880E+07 1.400 20800.0 NEC6OOH1-3O2=NEC6Q13-4 1.460E+09 1.100 33500.0 NEC6OOH1-4O2=NEC6Q14-1A 2.470E+06 1.500 20000.0 NEC6OOH1-4O2=NEC6Q14-3 4.010E+08 1.100 30100.0 NEC6OOH3-1O2=NEC6Q13-1A 7.130E+06 1.600 21000.0 NEC6OOH3-1O2=NEC6Q13-4 1.230E+06 1.500 20000.0 NEC6OOH3-4O2=NEC6Q34-1 3.700E+06 1.500 20000.0 NEC6OOH4-1O2=NEC6Q14-1A 7.130E+06 1.600 21000.0 NEC6OOH4-1O2=NEC6Q14-3 1.360E+07 1.300 18200.0 NEC6OOH4-3O2=NEC6Q34-1 4.320E+07 1.400 20800.0 NEC6Q11A-1B=¿C5H9A-AOOH+CH2O+OH 6.162E+13 0.000 27097.6 NEC6Q11A-3=¿C5H9B-AOOH+CH2O+OH 6.162E+13 0.000 27314.9 NEC6Q13-1A=¿C5H9A-COOH+CH2O+OH 3.081E+13 0.000 27177.1 NEC6Q13-1A=¿IC4H7OOH+CH3CHO+OH 3.081E+13 0.000 24639.3 NEC6Q14-1A=¿C5H9A-DOOH+CH2O+OH 3.081E+13 0.000 25337.8 NEC6Q34-1=¿IC4H8+HO2CH2CHO+OH 3.081E+13 0.000 24796.0 NEC6Q11A-4=IIC4H7Q2-T+C2H4 1.392E+14 0.000 19654.1 NEC6Q14-1A=IC4H7OOH+C2H4O2H 1.392E+14 0.000 27615.9 NEC6KET1-1A=NEC6KET1-1AO+OH 1.500E+16 0.000 40800.0 NEC6KET1-3=NEC6KET1-

3O+OH 1.050E+16 0.000 41800.0 NEC6KET1-4=NEC6KET1-4O+OH 1.500E+16 0.000 40800.0
NEC6KET3-1=NEC6KET3-1O+OH 1.500E+16 0.000 40800.0 NEC6KET3-4=NEC6KET3-4O+OH
1.500E+16 0.000 40800.0 NEC6KET4-1=NEC6KET4-1O+OH 1.500E+16 0.000 40800.0 NEC6KET4-
3=NEC6KET4-3O+OH 1.050E+16 0.000 41800.0 NEC6KET1-1AO=SC4H8CHO-2+CH2O 2.900E+12
0.380 11080.0 NEC6KET1-3O=IC3H6CHO+CH3CHO 2.900E+12 0.380 11080.0 NEC6KET1-4O=TC4H8CHO+CH
2.900E+12 0.380 11080.0 NEC6KET3-1O=IC5Y3-2J+CH2O 2.900E+12 0.380 11080.0 NEC6KET3-
4O=TC4H9CO+CH2O 2.900E+12 0.380 11080.0 NEC6KET4-1O=¿IC4H8+CH2O+HCO 2.900E+12
0.380 11080.0 NEC6KET4-3O=TC4H9CHO+HCO 2.900E+12 0.380 11080.0 NEC6Q13-4=NEC6D3-
1OOH+HO2 1.780E+12 0.240 15700.0 NEC6Q14-3=NEC6D3-1OOH+HO2 6.240E+10 0.720 15000.0
NEC6D3-1OOH=¿CC5H9-B+CH2O+OH 1.500E+16 0.000 40800.0 NEC6Q11A-1B=NEC6O11A-
1BOOH+OH 1.268E+12 0.000 16125.7 NEC6Q11A-3=NEC6O13-1AOOH+OH 1.902E+12 0.000
16011.7 NEC6Q11A-4=NEC6O14-1AOOH+OH 1.108E+11 0.000 8760.0 NEC6Q13-1A=NEC6O11A-
3OOH+OH 6.340E+11 0.000 16125.7 NEC6Q13-1A=NEC6O13-1AOOH+OH 6.340E+11 0.000
16726.1 NEC6Q13-4=NEC6O34-1OOH+OH 3.550E+12 0.000 10435.7 NEC6Q13-4=NEC6O14-
3OOH+OH 5.540E+10 0.000 8817.0 NEC6Q14-1A=NEC6O11A-4OOH+OH 6.340E+11 0.000 16125.7
NEC6Q14-1A=NEC6O14-1AOOH+OH 5.540E+10 0.000 8760.0 NEC6Q14-3=NEC6O13-4OOH+OH
9.510E+11 0.000 15722.8 NEC6Q14-3=NEC6O34-1OOH+OH 3.550E+12 0.000 8777.8 NEC6Q34-
1=NEC6O13-4OOH+OH 6.340E+11 0.000 16726.1 NEC6Q34-1=NEC6O14-3OOH+OH 5.540E+10
0.000 8760.0 NEC6O11A-1BOOH=¿AC5H9O-A2+CH2O+OH 1.500E+16 0.000 40800.0 NEC6O11A-
3OOH=¿IC4H7O+CH3CHO+OH 1.050E+16 0.000 41800.0 NEC6O11A-4OOH=¿IC4H7+2CH2O+OH
1.500E+16 0.000 40800.0 NEC6O13-1AOOH=¿AC5H9O-C+CH2O+OH 1.500E+16 0.000 40800.0
NEC6O13-4OOH=¿TC4H8CHO+CH2O+OH 1.500E+16 0.000 40800.0 NEC6O14-1AOOH=¿AC5H9O-
D+CH2O+OH 1.500E+16 0.000 40800.0 NEC6O14-3OOH=¿TC4H8CHO+CH2O+OH 1.050E+16
0.000 41800.0 NEC6O34-1OOH=¿B2E3M1OJ+CH2O+OH 1.500E+16 0.000 40800.0 NEC6O1-
1A+OH=¿AC5H10+HCO+H2O 2.500E+12 0.000 0.0 NEC6O1-1A+OH=¿SC3H5CHO+C2H5+H2O
2.500E+12 0.000 0.0 NEC6O1-3+OH=¿AC5H10+HCO+H2O 2.500E+12 0.000 0.0 NEC6O1-3+OH=¿IC4H8+CH3
2.500E+12 0.000 0.0 NEC6O1-4+OH=¿IC3H6CHO+C2H4+H2O 2.500E+12 0.000 0.0 NEC6O1-
4+OH=¿IC4H8+CH2CHO+H2O 2.500E+12 0.000 0.0 NEC6O3-4+OH=¿IC5D2Y4+CH3+H2O 2.500E+12
0.000 0.0 NEC6O3-4+OH=¿TC4H9+CH2CO+H2O 2.500E+12 0.000 0.0 NEC6O1-1A+HO2=¿AC5H10+HCO+H2
5.000E+12 0.000 17700.0 NEC6O1-1A+HO2=¿SC3H5CHO+C2H5+H2O2 5.000E+12 0.000 17700.0
NEC6O1-3+HO2=¿AC5H10+HCO+H2O2 5.000E+12 0.000 17700.0 NEC6O1-3+HO2=¿IC4H8+CH3CO+H2O2
5.000E+12 0.000 17700.0 NEC6O1-4+HO2=¿IC3H6CHO+C2H4+H2O2 5.000E+12 0.000 17700.0
NEC6O1-4+HO2=¿IC4H8+CH2CHO+H2O2 5.000E+12 0.000 17700.0 NEC6O3-4+HO2=¿IC5D2Y4+CH3+H2O2
5.000E+12 0.000 17700.0 NEC6O3-4+HO2=¿TC4H9+CH2CO+H2O2 5.000E+12 0.000 17700.0
IC4H7+CH2O=AC5H9O-D 6.880E+14 -0.890 7260.0 TC4H9CHO+O2=TC4H9CO+HO2 1.200E+05
2.500 37560.0 TC4H9CHO+OH=TC4H9CO+H2O 2.000E+06 1.800 -1300.0 TC4H9CHO+H=TC4H9CO+H2

4.140E+09 1.120 2320.0 TC4H9CHO+O=TC4H9CO+OH 5.940E+12 0.000 1868.0 TC4H9CHO+HO2=TC4H9CO-
4.090E+04 2.500 10200.0 TC4H9CHO+CH3=TC4H9CO+CH4 2.890E-03 4.620 3210.0 TC4H9CHO+CH3O=TC4H
1.000E+12 0.000 3300.0 TC4H9CHO+CH3O2=TC4H9CO+CH3O2H 4.090E+04 2.500 10200.0
TC4H9CHO+OH=TC4H8CHO+H2O 1.584E+10 0.970 1586.0 TC4H9CHO+HO2=TC4H8CHO+H2O2
7.137E+04 2.550 16490.0 TC4H9CHO+CH3O2=TC4H8CHO+CH3O2H 7.137E+04 2.550 16490.0
TC4H9CO=TC4H9+CO 1.000E+11 0.000 9600.0 XC6-1=XC6-2 1.510E+08 1.390 33000.0 DUP
XC6-1=XC6-2 1.730E+06 1.790 32500.0 DUP XC6OOH1-1A+O2=XC6D1-1AOOH+HO2 4.025E+00
3.320 4470.0 XC6OOH1-2+O2=XC6D1-1AOOH+HO2 2.650E+01 3.230 5330.0 XC6OOH1-2+O2=XC6D2-
1OOH+HO2 4.025E+00 3.320 4470.0 XC6OOH1-3+O2=XC6D1-4OOH+HO2 5.300E+01 3.230
5330.0 XC6OOH1-3+O2=XC6D2-1OOH+HO2 4.025E+00 3.320 4470.0 XC6OOH1-4+O2=XC6D1-
4OOH+HO2 4.025E+00 3.320 4470.0 XC6OOH2-3+O2=XC6D1-3OOH+HO2 5.300E+01 3.230
5330.0 XC6OOH2-4+O2=XC6D1-3OOH+HO2 4.025E+00 3.320 4470.0 XC6-1+H=XC6 1.000E+14
0.000 0.0 XC6-2+H=XC6 1.000E+14 0.000 0.0 CC5H11+CH3=XC6 1.000E+13 0.000 0.0 IC3H7+IC3H7=XC6
8.000E+12 0.000 0.0 XC6+H=XC6-1+H2 6.980E+05 2.690 6450.0 XC6+H=XC6-2+H2 1.204E+06
2.400 2583.0 XC6+O=XC6-1+OH 2.260E+14 0.000 7850.0 XC6+O=XC6-2+OH 7.940E+05 2.401
1150.0 XC6+OH=XC6-1+H2O 6.694E+06 2.078 375.6 XC6+OH=XC6-2+H2O 9.440E+10 0.576
-69.6 XC6+CH3=XC6-1+CH4 1.808E+00 3.650 7154.0 XC6+CH3=XC6-2+CH4 1.202E-09 6.360
893.0 XC6+HO2=XC6-1+H2O2 8.160E+01 3.590 17160.0 XC6+HO2=XC6-2+H2O2 1.300E+03
3.010 12090.0 XC6+CH3O2=XC6-1+CH3O2H 2.780E+00 3.970 18280.0 XC6+CH3O2=XC6-2+CH3O2H
5.240E+02 3.120 11100.0 XC6+CH3O=XC6-1+CH3OH 8.680E+11 0.000 6458.0 XC6+CH3O=XC6-
2+CH3OH 3.800E+10 0.000 2800.0 XC6+O2=XC6-1+HO2 8.400E+13 0.000 52800.0 XC6+O2=XC6-
2+HO2 1.400E+13 0.000 48000.0 XC6+C2H5=XC6-1+C2H6 2.000E+11 0.000 13400.0 XC6+C2H5=XC6-
2+C2H6 2.000E+11 0.000 7900.0 XC6+C2H3=XC6-1+C2H4 2.000E+12 0.000 18000.0 XC6+C2H3=XC6-
2+C2H4 4.000E+11 0.000 14300.0 XC6+O2CHO=XC6-1+HO2CHO 2.780E+00 3.970 18280.0
XC6+O2CHO=XC6-2+HO2CHO 5.240E+02 3.120 11100.0 XC6-1=CC5H10+CH3 2.887E+12 0.510
29826.4 XC6-1=C3H6+IC3H7 3.564E+17 -1.180 26229.5 XC6-2=BC5H10+CH3 1.590E+13 0.350
30649.2 XC6-1+O2=XC6D1+HO2 4.024E+00 3.320 10857.0 XC6-2+O2=XC6D1+HO2 5.289E+01
3.230 10591.8 XC6-2+O2=XC6D2+HO2 4.024E+00 3.320 10857.0 XC6D1+OH=XC6D1-1A+H2O
3.120E+06 2.000 -298.0 XC6D1+OH=XC6D1-3+H2O 6.140E+02 3.200 -3500.0 XC6D1+OH=XC6D1-
4+H2O 3.347E+06 2.078 375.6 XC6D2+OH=XC6D1-3+H2O 1.248E+07 2.000 -298.0 XC6D1+H=XC6D1-
1A+H2 1.730E+05 2.500 2492.0 XC6D1+H=XC6D1-3+H2 2.650E+06 2.200 0.0 XC6D1+H=XC6D1-
4+H2 3.490E+05 2.690 6450.0 XC6D2+H=XC6D1-3+H2 6.920E+05 2.500 2492.0 XC6D1+CH3=XC6D1-
1A+CH4 2.210E+00 3.500 5675.0 XC6D1+CH3=XC6D1-3+CH4 4.610E+00 3.100 2330.0 XC6D1+CH3=XC6D1-
4+CH4 9.040E-01 3.650 7154.0 XC6D2+CH3=XC6D1-3+CH4 8.840E+00 3.500 5675.0 XC6D1+HO2=XC6D1-
1A+H2O2 9.640E+03 2.600 13910.0 XC6D1+HO2=XC6D1-3+H2O2 1.810E+03 2.500 7154.0
XC6D1+HO2=XC6D1-4+H2O2 4.080E+01 3.590 17160.0 XC6D2+HO2=XC6D1-3+H2O2 3.856E+04

2.600 13910.0 XC6D1+CH3O=XC6D1-1A+CH3OH 9.000E+01 2.950 11990.0 XC6D1+CH3O=XC6D1-
3+CH3OH 1.000E+01 2.850 5231.0 XC6D1+CH3O=XC6D1-4+CH3OH 4.340E+11 0.000 6458.0
XC6D2+CH3O=XC6D1-3+CH3OH 3.600E+02 2.950 11990.0 XC6D1+CH3O2=XC6D1-1A+CH3O2H
9.640E+03 2.600 13910.0 XC6D1+CH3O2=XC6D1-3+CH3O2H 1.810E+03 2.500 7154.0 XC6D1+CH3O2=XC6D1
4+CH3O2H 1.390E+00 3.970 18280.0 XC6D2+CH3O2=XC6D1-3+CH3O2H 3.856E+04 2.600 13910.0
XC6D1+O2=XC6D1-1A+HO2 3.300E+12 0.000 39900.0 XC6D1+O2=XC6D1-3+HO2 1.100E+12
0.000 35220.0 XC6D1+O2=XC6D1-4+HO2 4.200E+13 0.000 52800.0 XC6D2+O2=XC6D1-3+HO2
1.320E+13 0.000 39900.0 XC6D1+O=XC6D1-1A+OH 4.410E+05 2.420 3150.0 XC6D1+O=XC6D1-
3+OH 3.300E+05 2.430 -790.0 XC6D1+O=XC6D1-4+OH 1.130E+14 0.000 7850.0 XC6D2+O=XC6D1-
3+OH 1.764E+06 2.420 3150.0 XC6D1+O2CHO=XC6D1-1A+HO2CHO 9.640E+03 2.600 13910.0
XC6D1+O2CHO=XC6D1-3+HO2CHO 1.810E+03 2.500 7154.0 XC6D1+O2CHO=XC6D1-4+HO2CHO
1.390E+00 3.970 18280.0 XC6D2+O2CHO=XC6D1-3+HO2CHO 3.856E+04 2.600 13910.0 B13DE2M+CH3=XC6
4 1.000E+11 0.000 7800.0 XC6-1=XC6D1+H 1.000E+13 0.000 36000.0 XC6-2=XC6D1+H 5.000E+12
0.000 43600.0 XC6-2=XC6D2+H 5.000E+12 0.000 43600.0 XC6D1+OH=XC6OH1-2J 1.000E+12
0.000 -1042.0 XC6D1+OH=XC6OH2-1J 1.000E+12 0.000 -1042.0 XC6D2+OH=XC6OH2-3J 2.000E+12
0.000 -1042.0 XC6OH1-2J+O2=XC6OH1-2O2 2.000E+12 0.000 0.0 XC6OH2-1J+O2=XC6OH2-
1O2 2.000E+12 0.000 0.0 XC6OH2-3J+O2=XC6OH2-3O2 2.000E+12 0.000 0.0 XC6OH1-2O2=¿IC5Y3+CH2O+O
2.500E+10 0.000 18860.0 XC6OH2-1O2=¿IC5Y3+CH2O+OH 2.500E+10 0.000 18860.0 XC6OH2-
3O2=¿CH3COCH3+CH3COCH3+OH 2.500E+10 0.000 18860.0 C3H4-A+IC3H7=XC6D1-1A 2.000E+11
0.000 7800.0 XC6D1-1A+HO2=XC6D1-1AO+OH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20
-2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -
4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33
-6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40
-8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / XC6D1-3+HO2=XC6D1-3O+OH
1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22
-3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -
5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970
14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670
21071.0 / XC6D1-1A+HO2=XC6D1-1AOOH 1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01
1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06 0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13
-1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15 -1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17
-2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18 -2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19
-2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / XC6D1-3+HO2=XC6D1-3OOH
1.000E+00 1.000 1.0 PLOG / 1.00E-02 2.050E+01 1.240 -22589.0 / PLOG / 1.00E-01 3.690E+06
0.080 -18331.0 / PLOG / 1.00E+00 2.020E+13 -1.450 -11709.0 / PLOG / 2.00E+00 1.490E+15
-1.870 -9604.0 / PLOG / 5.00E+00 1.850E+17 -2.310 -6991.0 / PLOG / 1.00E+01 2.880E+18

-2.550 -5260.0 / PLOG / 3.00E+01 3.450E+19 -2.710 -3140.0 / PLOG / 5.00E+01 5.330E+19 -2.700 -2438.0 / XC6D1-1A+CH3O2=XC6D1-1AO+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / XC6D1-3+CH3O2=XC6D1-3O+CH3O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / XC6D1-1A+C2H5O2=XC6D1-1AO+C2H5O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / XC6D1-3+C2H5O2=XC6D1-3O+C2H5O 1.000E+00 1.000 1.0 PLOG / 1.00E-02 6.900E+20 -2.680 229.0 / PLOG / 1.00E-01 4.500E+22 -3.180 1760.0 / PLOG / 1.00E+00 8.610E+27 -4.630 6415.0 / PLOG / 2.00E+00 1.920E+30 -5.280 8578.0 / PLOG / 5.00E+00 5.460E+33 -6.220 11879.0 / PLOG / 1.00E+01 2.980E+36 -6.970 14600.0 / PLOG / 3.00E+01 5.580E+40 -8.140 19040.0 / PLOG / 5.00E+01 4.440E+42 -8.670 21071.0 / XC6D1-4+O2=XC6D13+HO2 2.140E+00 3.710 7322.0 XC6D1-3+O2=XC6D13+HO2 2.140E+00 3.710 9322.0 XC6D13+OH=XC6D13-1AR+H2O 6.240E+06 2.000 -298.0 XC6D13+HO2=XC6D13-1AR+H2O2 3.460E-01 4.000 12103.0 C3H4-A+C3H5-S=XC6D13-1AR 1.000E+11 0.000 7800.0 XC6D1-3O=CH3+IC3H5COCH3 1.196E+16 -1.100 9941.0 XC6D1=AC5H9-C+CH3 1.000E+16 0.000 71000.0 XC6-1+O2=XC6-1O2 6.863E+16 -1.627 198.7 XC6-2+O2=XC6-2O2 9.752E+11 0.325 -417.3 XC6-1+HO2=XC6-1O+OH 9.000E+12 0.000 -1000.0 XC6-2+HO2=XC6-2O+OH 9.000E+12 0.000 -1000.0 XC6-1+CH3O2=XC6-1O+CH3O 9.000E+12 0.000 -1000.0 XC6-2+CH3O2=XC6-2O+CH3O 9.000E+12 0.000 -1000.0 XC6-1+XC6-1O2=XC6-1O+XC6-1O 9.000E+12 0.000 -1000.0 XC6-2+XC6-1O2=XC6-2O+XC6-1O 9.000E+12 0.000 -1000.0 XC6-1+XC6-2O2=XC6-1O+XC6-2O 9.000E+12 0.000 -1000.0 XC6-2+XC6-2O2=XC6-2O+XC6-2O 9.000E+12 0.000 -1000.0 XC6-1O2=XC6OOH1-1A 3.570E+06 1.600 21000.0 XC6-1O2=XC6OOH1-2 2.310E+09 0.800 27100.0 XC6-1O2=XC6OOH1-3 1.230E+07 1.200 15400.0 XC6-1O2=XC6OOH1-4 2.470E+06 1.500 20000.0 XC6-2O2=XC6OOH2-1 3.010E+09 1.200 33500.0 XC6-2O2=XC6OOH2-3 3.470E+10 0.400 26400.0 XC6-2O2=XC6OOH2-4 3.010E+08 1.100 21900.0 XC6-1O2=XC6D1+HO2 2.520E+08 1.320 27900.0 XC6-2O2=XC6D1+HO2 2.448E+10 0.890 29500.0 XC6-2O2=XC6D2+HO2 1.250E+13 0.020 29700.0 XC6-1O2+HO2=XC6-1OOH+O2 1.750E+10 0.000 -3275.0 XC6-2O2+HO2=XC6-2OOH+O2 1.750E+10 0.000 -3275.0 XC6-1O2+H2O2=XC6-

1OOH+HO2 2.400E+12 0.000 10000.0 XC6-2O2+H2O2=XC6-2OOH+HO2 2.400E+12 0.000 10000.0
XC6-1O2+XC6=XC6-1OOH+XC6-1 2.420E+13 0.000 20430.0 XC6-2O2+XC6=XC6-2OOH+XC6-
1 2.420E+13 0.000 20430.0 XC6-1O2+XC6=XC6-1OOH+XC6-2 4.040E+12 0.000 16000.0 XC6-
2O2+XC6=XC6-2OOH+XC6-2 4.040E+12 0.000 16000.0 XC6-1O2+CH3O2=¿XC6-1O+CH3O+O2
1.400E+16 -1.600 1860.0 XC6-2O2+CH3O2=¿XC6-2O+CH3O+O2 1.400E+16 -1.600 1860.0 XC6-
1O2+XC6-1O2=¿XC6-1O+XC6-1O+O2 1.400E+16 -1.600 1860.0 XC6-2O2+XC6-1O2=¿XC6-2O+XC6-
1O+O2 1.400E+16 -1.600 1860.0 XC6-2O2+XC6-2O2=¿XC6-2O+XC6-2O+O2 1.400E+16 -1.600
1860.0 XC6-1OOH=XC6-1O+OH 1.500E+16 0.000 41600.0 XC6-2OOH=XC6-2O+OH 6.000E+15
0.000 40800.0 XC6-1O=CH2O+CC5H11 5.500E+13 -0.210 18000.0 XC6-2O=CH3COCH3+IC3H7
2.460E+18 -1.280 17700.0 XC6-2O=CH3+IC5Y3 4.920E+18 -1.280 17700.0 XC6OOH1-1A=XC6O1-
1A+OH 6.340E+11 0.000 16125.7 XC6OOH1-2=XC6O1-2+OH 3.550E+12 0.000 8390.6 XC6OOH1-
3=XC6O1-3+OH 1.268E+12 0.000 14704.3 XC6OOH1-4=XC6O1-4+OH 5.540E+10 0.000 8760.0
XC6OOH2-1=XC6O1-2+OH 7.100E+12 0.000 11686.5 XC6OOH2-3=XC6O2-3+OH 3.550E+12
0.000 10629.3 XC6OOH2-4=XC6O1-3+OH 6.340E+11 0.000 17531.8 XC6OOH1-2=XC6D1+HO2
8.380E+09 0.920 14500.0 XC6OOH2-1=XC6D1+HO2 3.890E+13 -0.150 15500.0 XC6OOH2-3=XC6D2+HO2
3.010E+11 0.350 15200.0 XC6OOH1-3=C5H9B-AOOH+CH3 7.950E+12 0.350 30649.2 XC6OOH1-
1A=¿CC5H10+CH2O+OH 3.081E+13 0.000 25544.5 XC6OOH1-3=¿BC5H10+CH2O+OH 3.081E+13
0.000 25995.0 XC6OOH2-4=¿C3H6+CH3COCH3+OH 3.081E+13 0.000 23691.6 XC6OOH1-4=C3H6OOH1-
2+C3H6 1.392E+14 0.000 26384.7 XC6OOH1-4=C5H9C-AOOH+CH3 7.950E+12 0.350 30649.2
XC6OOH1-1A+O2=XC6OOH1-1AO2 3.430E+16 -1.627 198.7 XC6OOH1-2+O2=XC6OOH1-2O2
4.880E+11 0.325 -417.3 XC6OOH1-3+O2=XC6OOH1-3O2 4.880E+11 0.325 -417.3 XC6OOH1-
4+O2=XC6OOH1-4O2 3.430E+16 -1.627 198.7 XC6OOH2-1+O2=XC6OOH2-1O2 3.430E+16 -
1.627 198.7 XC6OOH2-3+O2=XC6OOH2-3O2 4.880E+11 0.325 -417.3 XC6OOH2-4+O2=XC6OOH2-
4O2 3.430E+16 -1.627 198.7 XC6OOH1-1AO2=XC6KET1-1A+OH 5.190E+04 1.900 18800.0 XC6OOH1-
2O2=XC6KET1-2+OH 3.660E+07 1.600 26900.0 XC6OOH1-3O2=XC6KET1-3+OH 1.650E+04
2.400 18900.0 XC6OOH1-4O2=XC6KET1-4+OH 4.770E+03 1.700 16600.0 XC6OOH1-1AO2=XC6D1-
1AOOH+HO2 2.520E+08 1.320 27900.0 XC6OOH1-2O2=XC6D1-1AOOH+HO2 1.224E+10 0.890
29500.0 XC6OOH1-2O2=XC6D2-1OOH+HO2 1.250E+13 0.020 29700.0 XC6OOH1-3O2=XC6D2-
1OOH+HO2 1.250E+13 0.020 29700.0 XC6OOH1-3O2=XC6D1-4OOH+HO2 2.448E+10 0.890
29500.0 XC6OOH1-4O2=XC6D1-4OOH+HO2 2.520E+08 1.320 27900.0 XC6OOH2-3O2=XC6D1-
3OOH+HO2 2.448E+10 0.890 29500.0 XC6OOH2-4O2=XC6D1-3OOH+HO2 2.520E+08 1.320
27900.0 XC6OOH1-1AO2=XC6Q11A-2 2.310E+09 0.800 27100.0 XC6OOH1-1AO2=XC6Q11A-3
1.230E+07 1.200 15400.0 XC6OOH1-1AO2=XC6Q11A-4 2.470E+06 1.500 20000.0 XC6OOH1-
2O2=XC6Q12-1A 1.510E+09 1.200 33500.0 XC6OOH1-2O2=XC6Q12-3 1.040E+11 0.400 26400.0
XC6OOH1-2O2=XC6Q12-4 3.010E+08 1.100 21900.0 XC6OOH1-3O2=XC6Q13-1A 1.500E+08 1.100
21900.0 XC6OOH1-3O2=XC6Q13-2 3.470E+10 0.400 26400.0 XC6OOH1-3O2=XC6Q13-4 3.010E+09

1.200 33500.0 XC6OOH1-4O2=XC6Q14-1A 1.230E+06 1.500 20000.0 DUP XC6OOH1-4O2=XC6Q14-2 1.230E+07 1.200 15400.0 DUP XC6OOH1-4O2=XC6Q14-2 2.310E+09 0.800 27100.0 DUP XC6OOH1-4O2=XC6Q14-1A 3.570E+06 1.600 21000.0 DUP XC6OOH2-1O2=XC6Q12-1A 3.570E+06 1.600 21000.0 XC6OOH2-1O2=XC6Q12-3 1.230E+07 1.200 15400.0 XC6OOH2-1O2=XC6Q12-4 2.470E+06 1.500 20000.0 XC6OOH2-3O2=XC6Q23-1 3.010E+08 1.100 21900.0 DUP XC6OOH2-3O2=XC6Q23-1 3.010E+09 1.200 33500.0 DUP XC6OOH2-4O2=XC6Q13-4 2.470E+06 1.500 20000.0 XC6OOH2-4O2=XC6Q13-2 2.310E+09 0.800 27100.0 XC6OOH2-4O2=XC6Q13-1A 3.570E+06 1.600 21000.0 XC6Q11A-3=¿C5H9B-DOOH+CH2O+OH 6.162E+13 0.000 27754.8 XC6Q12-4=¿C3KET21+C3H6+OH 3.081E+13 0.000 25599.8 XC6Q13-1A=¿AC3H5OOH+CH3COCH3+OH 3.081E+13 0.000 24841.4 XC6Q13-1A=¿C5H9C-BOOH+CH2O+OH 3.081E+13 0.000 26928.0 XC6Q14-1A=¿C5H9C-AOOH+CH2O+OH 3.081E+13 0.000 25544.5 XC6Q11A-4=C3H52-1,3OOH+C3H6 1.392E+14 0.000 24924.6 XC6Q14-1A=C3H6OOH1-2+AC3H5OOH 1.392E+14 0.000 28402.3 XC6KET1-1A=¿XC6KET1-1AO+OH 1.500E+16 0.000 40800.0 XC6KET1-2=¿XC6KET1-2O+OH 6.000E+15 0.000 41300.0 XC6KET1-3=¿XC6KET1-3O+OH 6.000E+15 0.000 41300.0 XC6KET1-4=¿XC6KET1-4O+OH 1.500E+16 0.000 40800.0 XC6KET1-1AO=¿DC5H9O-C+CH2O 2.900E+12 0.400 11080.0 XC6KET1-2O=¿IC5Y3+HCO 2.900E+12 0.400 11080.0 XC6KET1-3O=¿CH3CHCHO+CH3COCH3 2.900E+12 0.400 11080.0 XC6KET1-4O=¿SC4H8CHO-3+CH2O 2.900E+12 0.400 11080.0 XC6Q11A-2=XC6D1-1AOOH+HO2 1.676E+10 0.920 14500.0 XC6Q12-1A=XC6D1-1AOOH+HO2 1.350E+03 2.670 7900.0 XC6Q12-3=XC6D2-1OOH+HO2 1.860E+02 2.950 5400.0 XC6Q13-2=XC6D1-3OOH+HO2 8.380E+09 0.920 14500.0 XC6Q13-2=XC6D2-1OOH+HO2 1.860E+02 2.950 5400.0 XC6Q13-4=XC6D1-4OOH+HO2 3.890E+13 -0.150 15500.0 XC6Q14-2=XC6D1-4OOH+HO2 8.380E+09 0.920 14500.0 XC6Q23-1=XC6D1-3OOH+HO2 3.890E+13 -0.150 15500.0 XC6D1-1AOOH=¿C3H4-A+C2H5+CH2O+OH 8.520E+25 -3.610 27863.4 XC6D1-4OOH=¿AC5H9-C+CH2O+OH 1.500E+16 0.000 40800.0 XC6D1-3OOH=¿IC3H5COCH3+CH3+OH 6.000E+15 0.000 41300.0 XC6D2-1OOH=¿C4H6-2+CH2O2H+CH3 1.500E+16 0.000 40800.0 XC6D1-3OOH=¿C3H5-S+CH3COCH3+OH 6.000E+15 0.000 41300.0 XC6Q11A-2=XC6O12-1AOOH+OH 7.100E+12 0.000 8390.6 XC6Q11A-3=XC6O13-1AOOH+OH 2.536E+12 0.000 14704.3 XC6Q11A-4=XC6O14-1AOOH+OH 1.108E+11 0.000 8760.0 XC6Q12-1A=XC6O11A-2OOH+OH 6.340E+11 0.000 16163.7 XC6Q12-1A=XC6O12-1AOOH+OH 7.100E+12 0.000 11686.5 XC6Q12-3=XC6O13-2OOH+OH 1.268E+12 0.000 14871.5 XC6Q12-3=XC6O23-1OOH+OH 3.550E+12 0.000 10629.3 XC6Q12-4=XC6O14-2OOH+OH 5.540E+10 0.000 8760.0 XC6Q12-4=XC6O13-4OOH+OH 6.340E+11 0.000 17531.8 XC6Q13-1A=XC6O11A-3OOH+OH 6.340E+11 0.000 16125.7 XC6Q13-1A=XC6O13-1AOOH+OH 6.340E+11 0.000 17531.8 XC6Q13-2=XC6O12-3OOH+OH 3.550E+12 0.000 8390.6 XC6Q13-2=XC6O23-1OOH+OH 3.550E+12 0.000 10629.3 XC6Q13-4=XC6O14-2OOH+OH 5.540E+10 0.000 8817.0 XC6Q13-4=XC6O12-4OOH+OH 7.100E+12 0.000 11686.5 XC6Q14-1A=XC6O11A-4OOH+OH 6.340E+11 0.000 16125.7 XC6Q14-1A=XC6O14-1AOOH+OH 5.540E+10 0.000 8760.0 XC6Q14-2=XC6O12-4OOH+OH 3.550E+12 0.000 8390.6

XC6Q14-2=XC6O13-4OOH+OH 1.268E+12 0.000 14871.5 XC6Q23-1=XC6O12-3OOH+OH 7.100E+12
0.000 11686.5 XC6Q23-1=XC6O13-2OOH+OH 6.340E+11 0.000 17569.8 XC6O11A-2OOH=¿IC3H7COCH2+CH2O
6.000E+15 0.000 41300.0 XC6O11A-3OOH=¿C3H5O+CH3COCH3+OH 6.000E+15 0.000 41300.0
XC6O11A-4OOH=¿C4H71-3+2CH2O+OH 1.500E+16 0.000 40800.0 XC6O12-1AOOH=¿IC3H7COCH2+CH2O+O
1.500E+16 0.000 40800.0 XC6O12-3OOH=¿CH3COCH2+CH3COCH3+OH 6.000E+15 0.000 41300.0
XC6O12-4OOH=¿BC5H9O-A+CH2O+OH 1.500E+16 0.000 40800.0 XC6O13-1AOOH=¿B2E3M1OJ+CH2O+OH
1.500E+16 0.000 40800.0 XC6O13-2OOH=¿CH3CHCOC2H5+CH2O+OH 6.000E+15 0.000 41300.0
XC6O13-2OOH=¿CH3COCH2+CH3COCH3+OH 6.000E+15 0.000 41300.0 XC6O13-4OOH=¿CH2CH2COC2H5+O
1.500E+16 0.000 40800.0 XC6O14-1AOOH=¿CC5H9O-A+CH2O+OH 1.500E+16 0.000 40800.0
XC6O14-2OOH=¿CH2CH2COC2H5+CH2O+OH 6.000E+15 0.000 41300.0 XC6O23-1OOH=¿CH3CHCOC2H5+CH
1.500E+16 0.000 40800.0 XC6O1-1A+OH=¿AC5H10+HCO+H2O 5.000E+12 0.000 0.0 XC6O1-
2+OH=¿C4H72-2CHO+CH3+H2O 2.500E+12 0.000 0.0 XC6O1-3+OH=¿BC5H10+HCO+H2O
2.500E+12 0.000 0.0 XC6O1-4+OH=¿CH3CHCHO+C3H6+H2O 5.000E+12 0.000 0.0 XC6O2-
3+OH=¿IC3H5COCH3+CH3+H2O 5.000E+12 0.000 0.0 XC6O1-1A+HO2=¿AC5H10+HCO+H2O2
1.000E+13 0.000 17700.0 XC6O1-2+HO2=¿C4H72-2CHO+CH3+H2O2 5.000E+12 0.000 17700.0
XC6O1-3+HO2=¿BC5H10+HCO+H2O2 5.000E+12 0.000 17700.0 XC6O1-4+HO2=¿CH3CHCHO+C3H6+H2O2
1.000E+13 0.000 17700.0 XC6O2-3+HO2=¿IC3H5COCH3+CH3+H2O2 1.000E+13 0.000 17700.0
IC5Y3+OH=IC5Y3-1J+H2O 5.520E+02 3.120 -1176.0 IC5Y3+OH=IC5Y3-2J+H2O 4.680E+07
1.610 -35.0 IC5Y3+OH=IC3H7COCH2+H2O 5.280E+09 0.970 1586.0 IC5Y3+HO2=IC5Y3-1J+H2O2
3.440E+12 0.050 17880.0 IC5Y3+HO2=IC5Y3-2J+H2O2 9.640E+03 2.600 13910.0 IC5Y3+HO2=IC3H7COCH2+H
2.379E+04 2.550 16490.0 IC5Y3+CH3O2=IC5Y3-1J+CH3O2H 3.440E+12 0.050 17880.0 IC5Y3+CH3O2=IC5Y3-
2J+CH3O2H 9.640E+03 2.600 13910.0 IC5Y3+CH3O2=IC3H7COCH2+CH3O2H 2.379E+04 2.550
16490.0 C3H6+CH3CO=IC5Y3-1J 1.000E+11 0.000 6000.0 NC3H7+CH2CO=IC3H7COCH2 1.000E+11
0.000 6000.0 DC5H10O+OH=DC5H9O-C+H2O 4.680E+07 1.610 -35.0 DC5H10O+OH=DC5H9O-
B+H2O 5.280E+09 0.970 1586.0 DC5H10O+HO2=DC5H9O-C+H2O2 9.640E+03 2.600 13910.0
DC5H10O+HO2=DC5H9O-B+H2O2 2.379E+04 2.550 16490.0 DC5H10O+CH3O2=DC5H9O-C+CH3O2H
9.640E+03 2.600 13910.0 DC5H10O+CH3O2=DC5H9O-B+CH3O2H 2.379E+04 2.550 16490.0
SC3H5CHO+CH3=DC5H9O-C 1.000E+11 0.000 7800.0 IC4H8+HCO=DC5H9O-C 1.000E+11 0.000
6000.0 C3H6+CH2CHO=DC5H9O-B 1.000E+11 0.000 7800.0 DC5H10O+O2=IC4H9CO+HO2
1.200E+05 2.500 37560.0 DC5H10O+OH=IC4H9CO+H2O 2.000E+06 1.800 -1300.0 DC5H10O+H=IC4H9CO+H2
4.140E+09 1.120 2320.0 DC5H10O+O=IC4H9CO+OH 5.940E+12 0.000 1868.0 DC5H10O+HO2=IC4H9CO+H2O
4.090E+04 2.500 10200.0 DC5H10O+CH3=IC4H9CO+CH4 2.890E-03 4.620 3210.0 DC5H10O+CH3O=IC4H9CO-
1.000E+12 0.000 3300.0 DC5H10O+CH3O2=IC4H9CO+CH3O2H 4.090E+04 2.500 10200.0 IC4H9CO=IC4H9+CO
1.000E+11 0.000 9600.0 C4H72-2CHO=HCO+C4H72-2 1.000E+16 0.000 87000.0 IC3H5COCH3=SC3H5CO+CH3
1.000E+16 0.000 71000.0 L-C6H4+Hj=¿C-C6H4+H 1.400E+54 -11.700 34500.0 C-C6H4+Hj=¿C6H5
2.400E+60 -13.660 29500.0 L-C6H4+Hj=¿C6H5 1.700E+78 -19.720 31400.0 C6H3+Hj=¿L-C6H4

3.400E+43 -9.010 12120.0 L-C6H4+H¡=¿C6H3+H2 1.330E+06 2.530 9240.0 L-C6H4+OH¡=¿C6H3+H2O 3.100E+06 2.000 430.0 C6H2+H¡=¿C6H3 1.100E+30 -4.920 10800.0 C6H3+H¡=¿C6H2+H2 3.000E+13 0.000 0.0 C6H3+OH¡=¿C6H2+H2O 4.000E+12 0.000 0.0 C6H3+H¡=¿C4H2+C2H2 2.800E+23 -2.550 10780.0 C6H5+H=C6H6 4.170E+13 0.150 0.0 FULVENE=C6H5+H 2.570E+97 -23.160 153470.0 PLOG / 3.95E-02 2.570E+97 -23.160 153470.0 / PLOG / 1.00E+00 2.239E+68 -14.650 142570.0 / PLOG / 1.00E+01 8.511E+24 -4.970 113330.0 / FULVENE=C6H6 5.623E+81 -19.360 121500.0 PLOG / 3.95E-02 5.623E+81 -19.360 121500.0 / PLOG / 1.00E+00 1.445E+45 -8.900 96999.0 / PLOG / 1.00E+01 2.951E+31 -4.970 88465.0 / FULVENE+H=C6H6+H 3.630E+31 -4.748 18390.0 PLOG / 1.32E-01 4.324E+26 -3.446 12640.0 / PLOG / 1.00E+00 3.630E+31 -4.748 18390.0 / PLOG / 1.32E+00 1.839E+32 -4.931 19340.0 / PLOG / 1.32E+01 3.042E+36 -5.968 27480.0 / C6H6+H=C6H5+H2 1.420E+08 1.770 13055.9 C6H6+O2¡=¿C6H5+HO2 6.300E+13 0.000 63900.0 C6H6+O¡=¿C6H5+OH 3.100E+06 2.440 9140.0 C6H6+OH=C6H5+H2O 2.300E+04 2.683 733.3 C6H6+HO2=C6H5+H2O2 3.300E+12 0.000 28800.0 C6H6+CH3¡=¿C6H5+CH4 7.320E+12 0.000 18920.0 C6H6+CH3O2=C6H5+CH3O2H 4.119E+00 3.798 23067.1 C6H5+CH2O¡=¿C6H6+HCO 8.550E+04 2.190 38.0 C6H5+HCO¡=¿C6H6+CO 8.550E+04 2.190 38.0 C6H5=¿H+C4H2+C2H2 4.300E+12 0.620 77294.0 C6H6+OH=C6H5OH+H 1.325E+02 3.249 5590.0 C6H6+O=C6H5O+H 1.987E+07 1.800 3974.4 PLOG / 1.00E+01 1.987E+07 1.800 3974.4 / PLOG / 5.00E+01 3.553E+10 0.910 6323.3 / PLOG / 5.00E+02 1.325E+12 0.470 8435.7 / C6H6+O=C6H5OH 7.226E+22 -2.560 14995.4 PLOG / 1.00E-01 1.506E+29 -4.720 13344.0 / PLOG / 1.00E+00 7.226E+22 -2.560 14995.4 / PLOG / 1.00E+01 3.553E+24 -2.820 21906.9 / PLOG / 5.00E+01 5.841E+35 -5.890 34537.5 / PLOG / 5.00E+02 4.215E+31 -4.730 38432.4 / C6H6+O=C5H6+CO 6.022E+15 -0.490 14995.4 PLOG / 1.00E-01 7.226E+13 0.120 11778.1 / PLOG / 1.00E+00 6.022E+15 -0.490 14995.4 / PLOG / 1.00E+01 1.385E+38 -6.710 34634.9 / PLOG / 5.00E+01 1.566E+31 -4.730 33571.8 / PLOG / 5.00E+02 2.228E+56 -11.690 55603.8 / C6H6+O=C6H6O-24 2.288E+57 -14.620 15577.7 PLOG / 1.00E-01 7.226E+59 -16.060 14301.9 / PLOG / 1.00E+00 2.288E+57 -14.620 15577.7 / PLOG / 1.00E+01 1.385E+43 -9.650 13330.1 / PLOG / 5.00E+01 1.686E+38 -7.790 13511.0 / PLOG / 5.00E+02 1.144E+44 -9.060 20957.0 / DUP C6H6+O=C6H6O-24 1.204E+25 -3.720 9938.0 PLOG / 1.00E-01 2.288E+28 -4.970 9508.8 / PLOG / 1.00E+00 1.204E+25 -3.720 9938.0 / PLOG / 1.00E+01 2.830E+36 -6.770 18942.0 / PLOG / 5.00E+01 3.011E+28 -4.200 18411.4 / PLOG / 5.00E+02 4.155E+10 1.160 13228.8 / DUP C6H6+O=C6H6O-25 3.433E+28 -4.740 13240.7 PLOG / 1.00E-01 1.927E+27 -4.710 9508.8 / PLOG / 1.00E+00 3.433E+28 -4.740 13240.7 / PLOG / 1.00E+01 1.024E+46 -9.450 28383.2 / PLOG / 5.00E+01 2.228E+41 -10.500 40596.5 / PLOG / 5.00E+02 3.673E+38 -6.580 42555.9 / C6H5+HO2¡=¿C6H5O+OH 5.000E+12 0.000 0.0 C6H5O+OH¡=¿C6H5OOH 2.000E+13 0.000 0.0 C6H5+O2=C6H5O+O 8.570E+20 -2.270 7190.0 PLOG / 1.00E-01 9.820E+17 -1.470 4530.0 / PLOG / 1.00E+00 8.570E+20 -2.270 7190.0 / PLOG / 1.00E+01 7.940E+30 -4.980 16450.0 / PLOG / 1.00E+02 1.480E+44 -8.550 30130.0 /

C6H5+O2=¿C6H5OO 1.950E+11 0.420 -631.1 PLOG / 1.00E-01 6.690E+110 -32.750 14970.0 / PLOG / 1.00E+00 1.510E+136 -38.970 37550.0 / PLOG / 1.00E+01 2.110E+163 -45.730 63410.0 / PLOG / 1.00E+02 1.210E+181 -49.950 83430.0 / C6H5OO=¿C6H5+O2 3.240E+36 -7.200 50220.0 PLOG / 1.00E-01 1.450E+31 -6.030 45920.0 / PLOG / 1.00E+00 3.240E+36 -7.200 50220.0 / PLOG / 1.00E+01 3.090E+43 -8.780 57500.0 / PLOG / 1.00E+02 3.120E+42 -8.140 60270.0 / C6H5OO=C6H5O+O 3.700E+40 -8.440 45870.0 PLOG / 1.00E-01 2.490E+32 -6.520 38240.0 / PLOG / 1.00E+00 3.700E+40 -8.440 45870.0 / PLOG / 1.00E+01 7.980E+44 -9.270 52260.0 / PLOG / 1.00E+02 3.960E+38 -7.170 51380.0 / C6H5+O2=¿CJVCCVCCVO+CO 1.020E+14 -0.440 -1650.0 PLOG / 1.00E-01 1.128E+10 0.640 -5135.0 / PLOG / 1.00E+00 1.020E+14 -0.440 -1650.0 / PLOG / 1.00E+01 2.420E+27 -4.090 10380.0 / PLOG / 1.00E+02 9.800E+43 -8.560 26830.0 / C6H5OO=¿CJVCCVCCVO+CO 3.580E+50 -11.550 43310.0 PLOG / 1.00E-01 3.280E+45 -10.540 36300.0 / PLOG / 1.00E+00 3.580E+50 -11.550 43310.0 / PLOG / 1.00E+01 3.020E+47 -10.320 45110.0 / PLOG / 1.00E+02 8.880E+37 -7.340 42450.0 / C6H5OH=C6H5O+H 1.250E+67 -14.820 122641.0 PLOG / 1.00E-01 2.460E+91 -21.860 137144.0 / PLOG / 1.00E+00 1.250E+67 -14.820 122641.0 / PLOG / 1.00E+01 9.370E+66 -14.780 122572.0 / PLOG / 1.00E+02 7.630E+14 0.000 86900.0 / C6H4OH+H¡=¿C6H5OH 1.000E+14 0.000 0.0 C6H6O-24=C6H5OH 7.460E+74 -17.738 90359.0 PLOG / 1.00E+00 7.460E+74 -17.738 90359.0 / PLOG / 1.00E+01 2.760E+55 -12.012 80069.0 / PLOG / 1.00E+02 1.620E+11 0.633 50879.0 / C6H6O-24=C4D13KET 4.060E+57 -12.576 67450.0 PLOG / 1.00E+00 4.060E+57 -12.576 67450.0 / PLOG / 1.00E+01 1.600E+41 -7.815 57745.0 / PLOG / 1.00E+02 5.160E+12 0.314 38597.0 / C4D13KET=C5H6+CO 7.990E+65 -15.948 70413.0 PLOG / 1.00E+00 7.990E+65 -15.948 70413.0 / PLOG / 1.00E+01 1.830E+62 -14.493 73465.0 / PLOG / 1.00E+02 2.150E+11 0.231 42201.0 / C6H6O-25=¿C2H3+HCCO+C2H2 2.060E+105 -26.174 127274.0 PLOG / 1.00E+00 2.060E+105 -26.174 127274.0 / PLOG / 1.00E+01 5.050E+89 -21.220 123476.0 / PLOG / 1.00E+02 8.360E+14 0.313 76646.0 / C2H3+CJVCCVCVO=C4D13KET 1.000E+13 0.000 0.0 HCCO+C4H5-N=C4D13KET 1.000E+13 0.000 0.0 C2H2+HCCO=CJVCCVCVO 1.000E+13 0.000 0.0 C4D13KET+H=CVCCVCCJ+CO 1.000E+13 0.000 0.0 CJVCCVCVO+O2=¿C2H3CO+CO+C 2.453E+12 0.000 1041.2 CJVCCVCVO+O2=¿OVCCVCVO+H+CO 4.262E+11 0.000 -1537.1 CJVC-CVCVO+O2=OVCCVCVO+HCO 1.825E+11 0.000 -1537.1 OVCCVCVO+O2=¿HCCO+CO+HO2 1.000E+13 0.000 40700.0 OVCCVCVO+H=¿HCCO+CO+H2 1.340E+13 0.000 3300.0 OVCCVCVO+O=¿HCCO+C 5.940E+12 0.000 1868.0 OVCCVCVO+OH=¿HCCO+CO+H2O 9.240E+06 1.500 -962.0 OVC-CVCVO+HO2=¿HCCO+CO+H2O2 3.010E+12 0.000 11920.0 OVCCVCVO+CH3=¿HCCO+CO+CH4 2.608E+06 1.780 5911.0 OVCCVCVO+CH3O2=¿HCCO+CO+CH3O2H 1.505E+12 0.000 11920.0 C6H6O-24=C6H6O-B1 1.622E+64 -14.452 75948.0 PLOG / 1.00E+00 1.622E+64 -14.452 75948.0 / PLOG / 1.00E+01 1.978E+46 -9.230 65683.0 / PLOG / 1.00E+02 2.520E+12 0.442 43034.0 / C6H6O-25=C6H6O-B1 1.384E+65 -14.517 77116.0 PLOG / 1.00E+00 1.384E+65 -14.517 77116.0 / PLOG / 1.00E+01 9.760E+46 -9.231 66645.0 / PLOG / 1.00E+02 8.520E+12 0.485 43873.0 /

C6H6O-B1=C5H6+CO 6.780E+53 -11.662 51575.0 PLOG / 1.00E+00 6.780E+53 -11.662 51575.0 / PLOG / 1.00E+01 5.200E+48 -9.957 51544.0 / PLOG / 1.00E+02 2.280E+13 0.221 29390.0 / C6H6O-24=C6H5O+H 1.000E+16 0.000 71400.0 C6H6O-25=C6H5O+H 1.000E+16 0.000 73000.0 C6H6O-24+O2=C6H5O+HO2 2.000E+13 0.000 20300.0 C6H6O-24+H=C6H5O+H2 4.000E+07 1.738 2540.0 C6H6O-24+O=C6H5O+OH 1.475E+09 1.322 1547.1 C6H6O-24+OH=C6H5O+H2O 4.500E+05 2.110 -1400.0 C6H6O-24+HO2=C6H5O+H2O2 2.746E+00 3.798 1196.3 C6H6O-24+CH3=C6H5O+CH 1.746E+00 3.494 -1138.9 C6H6O-24+CH3O2=C6H5O+CH3O2H 1.373E+00 3.798 1196.3 C6H6O-25+O2=C6H5O+HO2 2.000E+13 0.000 21900.0 C6H6O-25+H=C6H5O+H2 4.000E+07 1.738 2540.0 C6H6O-25+O=C6H5O+OH 1.475E+09 1.322 1748.5 C6H6O-25+OH=C6H5O+H2O 4.500E+05 2.110 -1400.0 C6H6O-25+HO2=C6H5O+H2O2 2.746E+00 3.798 1990.2 C6H6O-25+CH3=C6H5O+CH4 1.746E+00 3.494 -663.8 C6H6O-25+CH3O2=C6H5O+CH3O2H 1.373E+00 3.798 1990.2 C6H5OH+O2=C6H5O+ 1.000E+13 0.000 38900.0 C6H5OH+H¡=¿C6H5O+H2 1.150E+14 0.000 12400.0 C6H5OH+O¡=¿C6H5O+OH 1.300E+13 0.000 2900.0 C6H5OH+OH=C6H5O+H2O 6.950E+07 1.400 -960.0 C6H5OH+HO2=C6H5O+H2O2 1.373E+00 3.798 10439.8 C6H5OH+CH3=C6H5O+CH4 8.732E-01 3.494 4392.4 C6H5OH+CH3O2=C6H5O+CH3 6.865E-01 3.798 10439.8 C6H5OH+C3H5-A¡=¿C6H5O+C3H6 4.900E+11 0.000 9400.0 C6H5OH+C4H5-I¡=¿C6H5O+C4H6 4.900E+11 0.000 9400.0 C6H5OH+C6H5¡=¿C6H5O+C6H6 4.900E+12 0.000 4400.0 C6H5OH+C6H5OO¡=¿C6H5O+C6H5OOH 1.330E+11 0.000 14000.0 C6H5OH+O2=C6H4OH+HO2 5.000E+13 0.000 64100.0 C6H5OH+H=C6H4OH+H2 1.183E+08 1.770 13055.9 C6H5OH+O¡=¿C6H4OH+OH 2.000E+13 0.000 14700.0 C6H5OH+OH=C6H4OH+H2O 2.629E+04 2.683 733.3 C6H5OH+HO2=C6H4OH+H2O 6.865E+00 3.798 23067.1 C6H5OH+CH3=C6H4OH+CH4 4.366E+00 3.494 11948.4 C6H5OH+CH3O2=C6H4OH- 3.433E+00 3.798 23067.1 C6H5OH+O=O-OC6H4OH+H 1.987E+07 1.800 3974.4 C6H5OH+O=P-OC6H4OH+H 1.987E+07 1.800 3974.4 C6H5OH+O=O-HOC6H4OH 7.226E+22 -2.560 14995.4 C6H5OH+O=P-HOC6H4OH 7.226E+22 -2.560 14995.4 O-HOC6H4OH=O-OC6H4OH+H 1.250E+67 -14.820 122641.0 P-HOC6H4OH=P-OC6H4OH+H 1.250E+67 -14.820 122641.0 O-HOC6H4OH+H=C6H5OH+OH 1.395E+05 2.533 3954.2 P-HOC6H4OH+H=C6H5OH+OH 1.395E+05 2.533 3954.2 HOC6H4CH3+OH=O-HOC6H4OH+CH3 4.697E+02 2.884 3221.3 HOC6H4CH3+OH=P-HOC6H4OH+CH3 3.132E+02 2.884 3221.3 O-HOC6H4OH+O2=O-OC6H4OH+HO2 2.000E+13 0.000 30600.0 O-HOC6H4OH+H=O-OC6H4OH+H2 2.300E+14 0.000 12400.0 O-HOC6H4OH+O=O-OC6H4OH+OH 2.600E+13 0.000 2900.0 O-HOC6H4OH+OH=O-OC6H4OH+H2O 1.390E+08 1.400 -960.0 O-HOC6H4OH+HO2=O-OC6H4OH+H2O2 2.746E+00 3.798 10439.8 O-HOC6H4OH+CH3=O-OC6H4OH+CH4 4.092E+00 3.469 4392.4 O-HOC6H4OH+CH3O2=O-OC6H4OH+CH3O2H 1.373E+00 3.798 10439.8 P-HOC6H4OH+O2=P-OC6H4OH+HO2 2.000E+13 0.000 34500.0 P-HOC6H4OH+H=P-OC6H4OH+H2 2.300E+14 0.000 12400.0 P-HOC6H4OH+O=P-OC6H4OH+OH 2.600E+13 0.000 2900.0 P-HOC6H4OH+OH=P-OC6H4OH+H2O 1.390E+08 1.400 -960.0 P-HOC6H4OH+HO2=P-OC6H4OH+H2O2 2.746E+00 3.798 10439.8 P-HOC6H4OH+CH3=P-OC6H4OH+CH4 4.092E+00 3.469 4392.4 P-HOC6H4OH+CH3O2=P-OC6H4OH+CH3O2H 1.373E+00 3.798 10439.8 C6H5O=C5H5+CO 3.562E+87 -21.565 91659.6

PLOG / 1.00E-02 2.212E+92 -23.753 86699.5 / PLOG / 5.00E-01 1.171E+90 -22.407 91919.9 /
PLOG / 1.00E+00 3.562E+87 -21.565 91659.6 / PLOG / 1.00E+01 4.812E+71 -16.658 85849.0 /
PLOG / 1.00E+02 1.309E+42 -7.958 69907.7 / C6H4OH+O2=O-OC6H4OH+O 8.570E+20 -2.270
7190.0 C6H4OH+O2=P-OC6H4OH+O 8.570E+20 -2.270 7190.0 C6H4OH+O2=¿O-OOC6H4OH
1.510E+136 -38.970 37550.0 C6H4OH+O2=¿P-OOC6H4OH 1.510E+136 -38.970 37550.0 O-OOC6H4OH=¿C6H4O
3.240E+36 -7.200 50220.0 P-OOC6H4OH=¿C6H4OH+O2 3.240E+36 -7.200 50220.0 O-OOC6H4OH=O-
OC6H4OH+O 3.700E+40 -8.440 45870.0 P-OOC6H4OH=P-OC6H4OH+O 3.700E+40 -8.440 45870.0
C6H4OH+O2=¿CO+C2H2+HCCOH+HCO 1.020E+14 -0.440 -1650.0 O-OOC6H4OH=¿CO+C2H2+HCCOH+HC
3.580E+50 -11.550 43310.0 P-OOC6H4OH=¿CO+C2H2+HCCOH+HCO 3.580E+50 -11.550 43310.0
C6H4OH+HO2=O-OC6H4OH+OH 5.000E+12 0.000 0.0 C6H4OH+HO2=P-OC6H4OH+OH 5.000E+12
0.000 0.0 O-OC6H4OH=O-C6H4O2+H 7.630E+14 0.000 71936.6 P-OC6H4OH=P-C6H4O2+H
7.630E+14 0.000 60013.4 O-OC6H4OH=C5H4OH+CO 1.400E+15 0.000 67000.0 DUP O-OC6H4OH=C5H4OH+C
9.900E+14 0.000 68900.0 DUP P-OC6H4OH=C5H4OH+CO 3.300E+14 0.000 58300.0 C6H5O+O2=O-
C6H4O2+OH 2.170E+07 1.300 17667.3 C6H5O+O2=P-C6H4O2+OH 2.170E+07 1.300 17667.3
C6H5O+O=O-C6H4O2+H 1.500E+14 0.000 0.0 C6H5O+O=P-C6H4O2+H 1.500E+14 0.000 0.0
O-C6H4O2¡=¿C5H4O+CO 1.000E+12 0.000 40000.0 P-C6H4O2¡=¿C5H4O+CO 3.700E+11 0.000
59000.0 P-C6H3O2+H¡=¿P-C6H4O2 1.000E+14 0.000 0.0 P-C6H4O2+H¡=¿P-C6H3O2+H2 2.000E+12
0.000 8100.0 P-C6H4O2+O¡=¿P-C6H3O2+OH 1.400E+13 0.000 14700.0 P-C6H4O2+OH¡=¿P-
C6H3O2+H2O 1.000E+06 2.000 4000.0 P-C6H4O2+H¡=¿C5H5O+CO 2.500E+13 0.000 4700.0 P-
C6H3O2+H=¿2C2H2+2CO 1.000E+14 0.000 0.0 P-C6H3O2+O=¿C2H2+HCCO+2CO 1.000E+14
0.000 0.0 C5H5+H=C5H6 3.158E+13 0.281 179.3 C5H6+O2=C5H5+HO2 2.000E+13 0.000 33400.0
C5H6+H=CYC5H71-3 6.540E+25 -3.510 8145.0 C5H6+CH3=C5H5CH3+H 8.110E+00 3.182 9383.0
C5H5CH3-1+H=C5H6+CH3 9.500E+05 2.000 944.0 C5H5CH3-2+H=C5H6+CH3 9.500E+05 2.000
944.0 C5H6+H=C5H5+H2 8.857E+07 1.847 3337.0 C5H6+O=C5H5+OH 1.750E+11 0.700 5884.0
C5H6+OH=C5H5+H2O 2.020E+06 2.200 -437.2 C5H6+HO2=C5H5+H2O2 3.910E-01 3.968 11701.5
C5H6+HCO=C5H5+CH2O 7.200E+06 1.900 17010.0 C5H6+CH3=C5H5+CH4 1.800E-01 4.000
0.0 C5H6+CH3O2=C5H5+CH3O2H 2.000E+12 0.000 15900.0 C5H6+C2H3=C5H5+C2H4 1.200E-
01 4.000 0.0 C5H6+C3H5-A=C5H5+C3H6 8.000E+11 0.000 13500.0 C5H6+C4H3-N=C5H5+C4H4
3.160E+11 0.000 16400.0 C5H6+C3H3=C5H5+C3H4-A 6.000E+12 0.000 12000.0 C5H6+C3H3=C5H5+C3H4-
P 6.000E+12 0.000 12000.0 C5H6+C4H5-N=C5H5+C4H6 6.000E+12 0.000 0.0 C5H6+C4H5-
I=C5H5+C4H6 6.000E+12 0.000 0.0 C5H6+C5H5O=C5H5+C5H5OH 1.000E+12 0.000 6000.0
C5H6+C6H5=C5H5+C6H6 6.000E+12 0.000 6000.0 C5H6+C2H3¡=¿C6H6+CH3 2.120E+67 -
16.080 42

!Toluene reactions taken from dayma

C4H5-N+C3H4-A=C6H5CH3+H 2.000E+11 0.00 3700.0 !(KERN 88) C4H5-N+C3H4-P=C6H5CH3+H

6.320E+11 0.00 3700.0 !(84COL/BIT*2) C3H3+C4H6=C6H5CH3+H 3.270E+05 1.28 -4611.0 !WANG ET AL., COMBUST.FLAME 212(2020)184-204

C6H5CH3=C6H5+CH3 1.400E+16 0.00 99800.0 !(92GLA/BRE) C6H5CH3=C6H5CH2+H 3.000E+15 0.00 88194.0 !(88MUL/COB*RTI*1.50)

!TOLUEN+H=C6H5CH2+H2 1.260E+14 0.00 8364.0 !(90HIP GP) C6H5CH3+H=C6H5CH2+H2 6.470E+00 3.98 3384.0 !OEHLSCHLAEGER ET AL., J.PHYS.CHEM.A 110(2006)9867-9873 !TOLUEN+H=C6H6+ 2.400E+13 0.00 5123.0 !(86ROB/TSA*DAG*2) C6H5CH3+H=C6H6+CH3 3.900E+08 1.25 2371.0 !WANG ET AL., COMBUST.FLAME 212(2020)184-204 C6H5CH3+CH3=C6H5CH2+CH4 8.880E+10 0.00 8754.0 !(FIT 201296) C6H5CH3+C2H5=C6H5CH2+C2H6 1.008E+11 0.00 9514.0 !(FITNIST) C6H5CH3+C6H5=C6H5CH2+C6H6 2.100E+12 0.00 4400.0 !(92EMD/BRE) C6H5CH3+C4H5-N=C6H5CH2+C4H6 4.000E+12 0.00 7500.0 !(RTI) C6H5CH3+C2H3=C6H5CH2+C2H4 4.000E+12 0.00 7500.0 !(RTI)

! CPT HIGH TEMPERATURE

!***UNIMOLECULAR DECOMPOSITION*** CPT¡=¿C5H10-1 1.26E16 0.00 84850 CPT¡=¿C2H4+C3H6 1.78E16 0.00 95070 CYC5H9+H¡=¿CPT 1E+14 0.00 0.00

!***H-ABSTRACTION*** CPT+H¡=¿CYC5H9+H2 6.50E+06 2.40 4471 2009. A/2 CPT+O2¡=¿CYC5H9+HO 1.00E+14 0.00 49640 CPT+HO2¡=¿CYC5H9+H2O2 3.16E+02 3.37 13720 CPT+CH3¡=¿CYC5H9+CH4 7.55 3.46 5481

CPT+C2H5¡=¿CYC5H9+C2H6 2.50E+11 0.00 10400

!***BETA-SCISSION*** CYC5H9¡=¿CYC5H8+H 8.84E+11 0.694 36624.5 ! ab initio computations CCSDT/PVTZ (MJR) PLOG/ 0.01 1.40E+66 -17 51500 / ! PLOGs calculated using Wang's falloff PLOG/ 0.1 2.40E+57 -14 49500 / ! DEG=4 PLOG/ 1 2.00E+55 -13 41000 / PLOG/ 5 2.40E+49 -11 50000 / PLOG/ 10 4.44E+49 -11 50800 / PLOG/ 20 1.320E+43 -9 48000 / CYC5H9¡=¿C5H91-5 1.24E+13 0.244 36044.4 ! ab initio computations CCSDT/PVTZ (MJR) PLOG/ 0.01 2.80E+74 -19.8 52500 / ! PLOGs calculated using Wang's falloff PLOG/ 0.1 2.20E+73 -19 55000 / ! DEG=2 PLOG/ 1 8.00E+62 -15.5 52500 / PLOG/ 5 2.40E+50 -11.5 48500 / PLOG/ 10 6.00E+45 -10 47300 / PLOG/ 20 2.40E+44 -9.5 47300 /

!***CYCLOPENTENE REACTIONS*** CYC5H8¡=¿C5H8D14 5.04E15 0.00 96850 CYC5H8¡=¿C5H81-3 5.06E15 0.00 6.6E+04 CYC5H8¡=¿C2H2+C3H6 7.12E15 0.00 107067 CYC5H8¡=¿C5H6+H2 2.24E13 0.0 60000 CYC5H8+H¡=¿CYC5H71-4+H2 1.3E+06 2.4 4.471E+03

CYC5H8+CH3¡=¿CYC5H71-4+CH4 1.51 3.5 5.481E+03

CYC5H8+C2H5¡=¿CYC5H71-4+C2H6 5E+10 0.0 10400 CYC5H8+H¡=¿CYC5H71-3+H2 6.752E+05 2.36 2.070E+02

CYC5H8+HO2¡=¿CYC5H71-3+H2O2 9.640E+03 2.55 1.053E+04 CYC5H8+CH3¡=¿CYC5H71-3+CH4 7.380E+00 3.31 4.002E+03

CYC5H8+C2H5¡=¿CYC5H71-3+C2H6 2.97 3.5 6637 ! BETA SCISSION OF CYCPENTYL RADICALS !C5H714-1¡=¿CYC5H71-4 9.6E8 1.05 5570 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA DECREASED BY 13.2 KCAL, ENERGY DIFF. BETWEEN VINYL-SEC AND SEC-SEC C-C BONDS !C5H6+H¡=¿CYC5H71-4 8.41E11 0.51 1230 ! ANALOGY WITH H+C3H6=IC3H7 CURRAN 2006 (DEG=2) !CVCCVCCJ¡=¿CYC5H71-3 6.14E10 1.05 23850 ! MATHEU ET AL. 2002 1,5 ENDO ADDITION. EA INCREASED BY 8.05 KCAL, THE STABILIZATION ENERGY OF DOUBLE RESONANCE COMPARED TO SINGLE RES. !C5H6+H¡=¿CYC5H71-3 8.48E+11 0.51 1230 ! ANALOGY WITH H+C3H6=IC3H7 CURRAN 2006 (DEG=2) !RADICAL ASSOCIATION CYC5H71-4+H¡=¿CYC5H8 1E14 0.00 0.0 CYC5H71-3+H¡=¿CYC5H8 5.83E13 0.176 125

!ADDITION

CPT1Q2J=CPT1Q3J 4.62E-31 12.01 8911.0 PLOG/9.869E-04 4.74E-68 23.10 -8066.0/ ! fit btw. 300 and 460 K with MAE of 1.2PLOG/9.869E-03 8.44E-106 35.98 -15440.0/ ! fit btw. 300 and 500 K with MAE of 2.5PLOG/9.869E-02 5.84E-113 38.51 -16100.0/ ! fit btw. 300 and 550 K with MAE of 5.0PLOG/9.869E-01 8.78E-86 29.58 -8633.0/ ! fit btw. 300 and 650 K with MAE of 8.6PLOG/9.869E+00 1.11E-50 18.23 1779.0/ ! fit btw. 300 and 800 K with MAE of 10.3PLOG/9.869E+01 4.62E-31 12.01 8911.0/ ! fit btw. 300 and 1000 K with MAE of 4.2

CPT1Q2J=PT1N3Q5J 2.30E-05 5.09 26950.0 PLOG/9.869E-04 2.08E-05 4.80 33470.0/ ! fit btw. 300 and 460 K with MAE of 0.4PLOG/9.869E-03 6.69E-03 4.30 34460.0/ ! fit btw. 300 and 500 K with MAE of 1.1PLOG/9.869E-02 5.67E+05 1.97 36830.0/ ! fit btw. 300 and 550 K with MAE of 1.9PLOG/9.869E-01 5.79E+12 -0.05 39230.0/ ! fit btw. 300 and 650 K with MAE of 2.7PLOG/9.869E+00 2.55E-35 14.87 22260.0/ ! fit btw. 300 and 800 K with MAE of 18.4PLOG/9.869E+01 2.30E-05 5.09 26950.0/ ! fit btw. 300 and 1000 K with MAE of 16.2

CPT1Q2J=PT1N1Q5J 1.14E-03 4.65 28770.0 PLOG/9.869E-04 1.60E-05 5.03 35070.0/ ! fit btw. 300 and 460 K with MAE of 0.6PLOG/9.869E-03 2.81E+00 3.59 36630.0/ ! fit btw. 300 and 500 K with MAE of 1.2PLOG/9.869E-02 2.02E+09 0.95 39210.0/ ! fit btw. 300 and 550 K with MAE of 2.0PLOG/9.869E-01 2.93E+16 -1.12 41650.0/ ! fit btw. 300 and 650 K with MAE of 2.8PLOG/9.869E+00 1.06E-23 11.38 27910.0/ ! fit btw. 300 and 800 K with MAE of 20.4

!MCP ————————Start from here————————MCP !**********CLASS 1 - UNIMOLECULAR FUEL DECOMPOSITION**********! ! !MCP = C6H12-1 6.714e+15

0.00 8.284e+04 !Dayma, Int.J.Chem.Kinet., 1(2020) !MCP = C6H12-2 1.679e+15 0.00 8.284e+04 !Dayma, Int.J.Chem.Kinet., 1(2020) !MCP = IC6D1 2.518e+15 0.00 8.484e+04 !Dayma, Int.J.Chem.Kinet., 1(2020) !MCP = I3C6D1 2.518e+15 0.00 8.484e+04 !Dayma, Int.J.Chem.Kinet., 1(2020) !MCP = IC6D4 2.518e+15 0.00 8.484e+04 !Dayma, Int.J.Chem.Kinet., 1(2020)

! THIS WORK (Ring opening isomerization)

MCP = INT1 4.43E+15 0.0 91764.9 MCP = INT2 6.11E+15 0.0 91248.2 MCP = INT3 6.81E+14 0.0 90258.6

INT1 = C6H12-1 2.83E+12 0.0 5236.5 INT1 = C6H12-2 1.78E+12 0.0 4573.5 INT2 = IC6D4 3.76E+11 0.0 3392.9 INT2 = IC6D1 8.57E+11 0.0 4841.6 INT3 = I3C6D1 8.33E+11 0.0 5144.3

!C-CH3 DISSOCIATION

MCP = CYC5H9+CH3 3.40E+14 0.0 81331.9 ! THIS WORK

!MCP = CYC5H9+CH3 1.100e+27 -3.20 8.639e+04 !Zhang et al., Energy Fuels, 27(2013)1679-1687 ! PLOG / 0.197 1.500e+80 -18.67 1.169e+05 / ! PLOG / 0.395 8.650e+63 -13.89 1.082e+05 / ! PLOG / 1 5.930e+64 -14.15 1.085e+05 / ! PLOG / 10 3.590e+45 -8.56 9.743e+04 / ! PLOG / 100 1.660e+33 -4.99 9.010e+04 /

MCPR1+H¡=¿MCP 5.2E+12 0.28 0 !Harding's 2005 h+tertiary rad MCPR2+H¡=¿MCP 1.7E+13 0.22 0 !Harding's 2005 H+SECONDARY rad MCPR3+H¡=¿MCP 1.7E+13 0.22 0 !Harding's 2005 H+SECONDARY rad CPTCH2+H¡=¿MCP 5.4E+13 0.16 0 !Harding's 2005 H+PRIMARY rad ! !**********CLASS 2 - H ABSTRACTION FOR MCP **********! ! !THIS WORK

MCP+CH3 = CPTCH2+CH4 3.26E+13 0.0 19829.5 MCP+CH3 = MCPR2+CH4 1.21E+13 0.0 17161.5 MCP+CH3 = MCPR3+CH4 1.25E+13 0.0 16810.7 MCP+CH3 = MCPR1+CH4 3.80E+12 0.0 15000.0

MCP+H= CPTCH2+H2 4.59E+14 0.0 13436.9 MCP+H = MCPR2+H2 1.76E+14 0.0 9914.3 MCP+H = MCPR3+H2 1.76E+14 0.0 9815.0 MCP+H = MCPR1+H2 5.14E+13 0.0 7921.4

!**********MCPR1**********

!MCP+H¡=¿MCPR1+H2 5.43E+05 2.36 2887 !Tian et al., EnergyFuels, 29(2015)428-441

!MCP+CH3¡=¿MCPR1+CH4 6.01E-10 6.36 893 !Sarathy 2011 rate rule

!**********MCPR2**********

!MCP+H¡=¿MCPR2+H2 3.11E+05 2.57 4359 !Tian et al., EnergyFuels, 29(2015)428-441

!MCP+CH3¡=¿MCPR2+CH4 3.02E+00 3.46 5481 !Sarathy 2011 rate rule

!**********MCPR3**********

!MCP+H¡=¿MCPR3+H2 2.97E+05 2.59 4138 !Tian et al., EnergyFuels, 29(2015)428-441

!MCP+CH3¡=¿MCPR3+CH4 3.02E+00 3.46 5481 !Sarathy 2011 rate rule

!**********CPTCH2**********
!MCP+H¡=¿CPTCH2+H2 1.68E+05 2.61 6535 !Tian et al., EnergyFuels, 29(2015)428-441

!MCP+CH3¡=¿CPTCH2+CH4 4.53E-01 3.65 7154 !Sarathy 2011 rate rule

! !********** CLASS 3 - CYCLIC C6H11 radical decomposition **********!already calculated in this paper ! !MCPR1¡=¿MCYC5-1N+H 3.00E+13 0.00 39000 MCPR1=MCYC5-1N+H 4.91E+16 0.0 40290.4 !OUR CALCULATION

!MCPR1¡=¿MCYC5-1N+H 4.17E+07 1.85 37481 ! calculated in this work ! PLOG / 0.001 5.06E+10 0.29 35896 / ! 800 K-2000 K !PLOG / 0.01 3.72E+10 0.52 36620 / ! 800 K-2000 K ! PLOG / 0.1 5.44E+09 0.94 37014 / ! 800 K-2000 K !PLOG / 1 7.91E+08 1.32 37253 / ! 800 K-2000 K !PLOG / 10 1.87E+09 1.23 37474 / ! 800 K-2000 K !PLOG / 100 3.26E+09 1.18 37654 / ! 800 K-2000 K !MCPR1¡=¿MCYC5-2N+H 6.00E+13 0.00 38000 MCPR1=MCYC5-2N+H 7.78E+17 0.0 41337.5 !OUR CALCULATION

!MCPR1¡=¿MCYC5-2N+H 1.41E+08 1.58 34371 ! calculated in this work !PLOG / 0.001 4.97E+10 0.32 33209 / ! 800 K-2000 K !PLOG / 0.01 3.61E+10 0.51 33749 / ! 800 K-2000 K ! PLOG / 0.1 7.27E+09 0.85 34041 / ! 800 K-2000 K !PLOG / 1 1.23E+09 1.18 34190 / ! 800 K-2000 K !PLOG / 10 4.22E+09 1.03 34417 / ! 800 K-2000 K !PLOG / 100 7.35E+09 0.98 34565 / ! 800 K-2000 K !MCPR2¡=¿MCYC5-2N+H 1.50E+13 0.00 37500

MCPR2=MCYC5-2N+H 1.39E+13 0.0 34965.2 !OUR CALCULATION

!MCPR2¡=¿MCYC5-2N+H 1.18E+08 1.68 34248 ! calculated in this work ! PLOG / 0.001 3.85E+10 0.04 31763 / ! 800 K-2000 K !PLOG / 0.01 4.43E+10 0.26 32582 / ! 800 K-2000 K ! PLOG / 0.1 2.98E+10 0.53 33310 / ! 800 K-2000 K !PLOG / 1 1.95E+10 0.71 33752 / ! 800 K-2000 K !PLOG / 10 2.62E+09 1.11 33997 / ! 800 K-2000 K !PLOG / 100 1.67E+09 1.23 34199 / ! 800 K-2000 K !MCPR2¡=¿MCYC5-3N+H

MCPR2=MCYC5-3N+H 4.13E+14 0.0 37689.4 !OUR CALCULATION

!MCPR2¡=¿MCYC5-3N+H 4.81E+07 1.81 36337 ! calculated in this work !PLOG / 0.001 3.93E+10 -0.14 33326 / ! 800 K-2000 K !PLOG / 0.01 4.56E+10 0.15 34304 / ! 800 K-2000 K !PLOG / 0.1 2.48E+10 0.49 35164 / ! 800 K-2000 K ! PLOG / 1 1.41E+10 0.72 35670 / ! 800 K-2000 K ! PLOG / 10 1.71E+09 1.15 35997 / ! 800 K-2000 K !PLOG / 100 8.36E+08 1.32 36224 / ! 800 K-2000 K !MCPR2(+M)¡=¿CYC5H8+CH3(+M) 1.76E+11 0.57 28791.6 MCPR2=CYC5H8+CH3 3.81E+14 0.0 32441.7 !OUR CALCULATION

!LOW / 4.70E-39 16.77 -603.1 / !TROE / -27.89 216 28 50000.0 / !H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ !MCPR2¡=¿CYC5H8+CH3 1.22E+09 1.57 31152 ! calculated in this work !PLOG / 0.001 3.31E+10 0.50 29183 / ! 800 K-2000 K !PLOG / 0.01 2.99E+10 0.69 29754 / ! 800 K-2000 K !PLOG / 0.1 3.73E+10 0.81 30364 / ! 800 K-2000 K ! PLOG / 1 2.47E+10 0.97 30694 / ! 800 K-2000 K !PLOG / 10 6.11E+09 1.25 30905 / ! 800 K-2000 K !PLOG / 100 5.47E+09 1.31 31068 / ! 800 K-2000 K !MCPR3¡=¿MCYC5-3N+H 3.00E+13 0.00 38000 MCPR3=MCYC5-3N+H 2.06E+14 0.0 37500.7 !OUR CALCULATION

!MCPR3¡=¿MCYC5-3N+H 4.96E+07 1.76 35949 ! calculated in this work !PLOG / 0.001 5.11E+10 0.33 34790 / ! 800 K-2000 K !PLOG / 0.01 2.15E+10 0.61 35289 / ! 800 K-2000 K !PLOG / 0.1 2.92E+09 1.00 35540 / ! 800 K-2000 K !PLOG / 1 3.81E+09 1.02 35781 / ! 800 K-2000 K !PLOG / 10 1.91E+09 1.16 35918 / ! 800 K-2000 K !PLOG / 100 9.78E+09 0.95 36152 / ! 800 K-2000 K !MCPR3¡=¿MCYC5-4N+H 3.00E+13 0.00 38000 MCPR3=MCYC5-4N+H 4.14E+15 0.0 37858.3 !our calculation

!MCPR3¡=¿MCYC5-4N+H 5.93E+07 1.75 35792 ! calculated in this work !PLOG / 0.001 4.94E+10 0.35 34633 / ! 800 K-2000 K !PLOG / 0.01 2.37E+10 0.60 35140 / ! 800 K-2000 K ! PLOG / 0.1 3.03E+09 1.00 35373 / ! 800 K-2000 K !PLOG / 1 4.18E+09 1.01 35617 / ! 800 K-2000 K !PLOG / 10 1.88E+09 1.17 35734/ ! 800 K-2000 K !PLOG / 100 1.07E+10 0.94 35983 / ! 800 K-2000 K !CPTCH2¡=¿MCYC5-1N+H 1.50E+13 0.00 37500

CPTCH2=MCYC5-1N+H 2.50E+12 0.0 36843.0 !OUR CALCULATION

!CPTCH2¡=¿MCYC5-1N+H 4.24E+06 1.79 35619 ! calculated in this work !PLOG / 0.001 5.26E+09 0.52 35207 / ! 800 K-2000 K !PLOG / 0.01 1.07E+09 0.85 35506 / ! 800 K-2000 K !PLOG / 0.1 7.67E+08 0.96 35732 / ! 800 K-2000 K !PLOG / 1 1.04E+09 0.96 35952 / ! 800 K-2000 K !PLOG / 10 3.99E+08 1.13 35993 / ! 800 K-2000 K !PLOG / 100 1.41E+08 1.27 35892 / ! 800 K-2000 K ! !********** CLASS 4 - CYCLIC C6H11 RADICAL ISOMERIZATION **********! ! CPTCH2¡=¿MCPR3 9.550e-02 3.40 1.5367e+04 !Gong et al., EnergyFuels 26(2012)2811-2820 ! !********** CLASS 5 - CYCLIC C6H11 RADICAL ISOMERIZATION(IOSMERIZATIONS) **********! ! !CPTCH2=C6H111-6 2.750e+09 0.991 2.326e+04

CPTCH2=C6H111-6 1.51E+12 0.0 23381.029 !OUR CALCULATION

!CPTCH2=C6H111-6 4.03E+08 1.13 22209 ! calculated in this work !PLOG / 1 7.19E+03 2.50 20410 / ! 800 K-2000 K !PLOG / 10 1.92E+05 2.14 21055 / ! 800 K-2000 K ! PLOG / 100 3.36E+07 1.44 21762 / ! 800 K-2000 K !MCPR1=IC6D1-5 1.860e+12 0.419 3.437e+04 MCPR1=IC6D1-5 3.03E+16 0.0 38494.2 !OUR CALCULATION

!MCPR1=IC6D1-5 4.95E+08 1.37 32335 ! calculated in this work !PLOG / 0.01 2.09E+07 1.45 30675 / ! 800 K-2000 K !PLOG / 0.1 1.84E+07 1.66 31298 / ! 800 K-2000 K !PLOG / 1 4.65E+07 1.62 31704 / ! 800 K-2000 K !PLOG / 10 2.49E+08 1.42 32049 / ! 800 K-2000 K !PLOG / 100 9.13E+09 0.93 32462 / ! 800 K-2000 K !MCPR2(+M)=I3C6D1-6(+M) 3.55E+12 0.15 32404.0 ! 08/TSAwip !!!! CH3-4-P5XC5H8–¿PXCH2-4-1C5H9 ! LOW / 1.90E-36 15.96 -578.8 / ! TROE / -11.13 269 28 50000.0 / !H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/

MCPR2=I3C6D1-6 3.44E+12 0.0 34569.8 !OUR CALCULATION

!MCPR2=I3C6D1-6 2.51E+08 1.54 32322 ! calculated in this work !PLOG / 0.01 4.43E+07 1.35 30541 / ! 800 K-2000 K !PLOG / 0.1 6.79E+07 1.48 31233 / ! 800 K-2000 K !PLOG / 1 4.15E+08 1.30 31688 / ! 800 K-2000 K !PLOG / 10 4.06E+09 1.02 32061 / ! 800 K-2000 K !PLOG / 100 2.48E+09 1.15 32278 / ! 800 K-2000 K !MCPR2(+M)=C6H112-6(+M) 7.59E+11 0.15 32940.5 ! 08/TSAwip ! LOW / 1.10E-36 16.19 -602.5 / ! TROE / -21.6 225 28 50000.0 / !H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/

MCPR2=C6H112-6 7.78E+13 0.0 34571.8 !OUR CALCULATION

!MCPR2=C6H112-6 1.06E+08 1.97 32796 ! calculated in this work !PLOG / 0.001 4.84E+06 1.89 30657 / ! !PLOG / 0.01 2.68E+07 1.83 31419 / ! 800 K-2000 K !PLOG / 0.1 5.08E+08 1.47 31874 / ! 800 K-2000 K !PLOG / 1 1.82E+09 1.37 32264 / ! 800 K-2000 K !PLOG / 10 2.41E+09 1.40 32571 / ! 800 K-2000 K !PLOG / 100 1.54E+09 1.52 32773 / ! 800 K-2000 K !MCPR3=IC6D4-1 6.760e+11 0.692 3.545e+04 MCPR3=IC6D4-1 9.89E+12 0.0 35078.5 !OUR CALCULATION

!MCPR3=IC6D4-1 1.68E+08 1.57 33249 ! calculated in this work !PLOG / 0.01 8.60E+06 1.63 31637 / ! 800 K-2000 K !PLOG / 0.1 9.67E+06 1.80 32268 / ! 800 K-2000 K !PLOG / 1 3.28E+07 1.70 32682 / ! 800 K-2000 K !PLOG / 10 8.44E+08 1.26 33084 / ! 800 K-2000 K !PLOG / 100 3.53E+09 1.10 33369 / ! 800 K-2000 K !MCPR3=C6H111-5 1.440e+13 0.277 3.374e+04 MCPR3=C6H111-5 6.34E+13 0.0 34238.0 !OUR CALCULATION

!MCPR3=C6H111-5 5.22E+08 1.43 32048 ! calculated in this work !PLOG / 0.01 8.05E+06 1.77 30732 / ! 800 K-2000 K !PLOG / 0.1 8.85E+07 1.52 31231 / ! 800 K-2000 K !PLOG / 1

2.11E+08 1.47 31588 / ! 800 K-2000 K !PLOG / 10 1.23E+09 1.25 31880 / ! 800 K-2000 K !PLOG / 100 8.06E+10 0.66 32309 / ! 800 K-2000 K !

! ! !********** CLASS 6 - CYCLIC C6H10 ABSTRACTION **********!

!Adopted by Fridlyand et al. CNF, 2019, 200, 387-404 MCYC5-1N+H¡=¿MCYC51N3J+H2 6.75E+05 2.36 207 MCYC5-1N+CH3¡=¿MCYC51N3J+CH4 7.38E+00 3.31 4002

MCYC5-1N+C2H5¡=¿MCYC51N3J+C2H6 2.97 3.5 6637 MCYC51N3J+H¡=¿MCYC5-1N 5.83E13 0.176 125 MCYC5-2N+H¡=¿MCYC51N3J+H2 5.064E+05 2.360 2.070E+02

MCYC5-2N+CH3¡=¿MCYC51N3J+CH4 5.535E+00 3.310 4.002E+03

MCYC5-2N+C2H5¡=¿MCYC51N3J+C2H6 1.67 3.5 6637 MCYC5-2N+H¡=¿MCYC52N6J+H2 3.376E+05 2.360 2.070E+02

MCYC5-2N+CH3¡=¿MCYC52N6J+CH4 3.69E+00 3.310 4.002E+03

MCYC5-2N+C2H5¡=¿MCYC52N6J+C2H6 1.485 3.5 6637 MCYC5-2N+H¡=¿MCYC52N4J+H2 3.376E+05 2.360 2.070E+02

MCYC5-2N+CH3¡=¿MCYC52N4J+CH4 3.69E+00 3.310 4.002E+03

MCYC5-2N+C2H5¡=¿MCYC52N4J+C2H6 1.485 3.5 6637 MCYC51N3J+H¡=¿MCYC5-2N 5.83E13 0.176 125 MCYC52N6J+H¡=¿MCYC5-2N 5.83E13 0.176 125 MCYC52N4J+H¡=¿MCYC5-2N 5.83E13 0.176 125 MCYC5-3N+H¡=¿MCYC52N4J+H2 1.688E+05 2.36 2.070E+02

MCYC5-3N+CH3¡=¿MCYC52N4J+CH4 1.845E+00 3.31 4.002E+03

MCYC5-3N+C2H5¡=¿MCYC52N4J+C2H6 7.425E-01 3.5 6.637E+03 MCYC5-3N+H¡=¿MCYC54N3J+H2 3.376E+05 2.360 2.070E+02 MCYC5-3N+CH3¡=¿MCYC54N3J+CH4 3.69E+00 3.31 4.002E+03

MCYC5-3N+C2H5¡=¿MCYC54N3J+C2H6 1.485 3.5 6.637E+03 MCYC54N3J+H¡=¿MCYC5-3N 5.83E13 0.176 125 MCYC5-4N+H¡=¿MCYC54N3J+H2 6.752E+05 2.360 2.070E+02 MCYC5-4N+CH3¡=¿MCYC54N3J+CH4 7.380E+00 3.310 4.002E+03

MCYC5-4N+C2H5¡=¿MCYC54N3J+C2H6 2.97 3.5 6637 MCYC54N3J+H¡=¿MCYC5-4N 5.83E13 0.176 125 ! !********** CLASS 7 - CYCLIC C6H10 ISOMERIZATION **********! ! !Adopted by Fridlyand et al. CNF, 2019, 200, 387-404 MCYC5-1N¡=¿C6H101-5 5.04E15 0.00 93280 !analogy with cyc5h8¡=¿c5h81-4. Ea REDUCED by 3.57kcal (diff. IN BDE OF VIN AND VINS). MCYC5-1N¡=¿C4H6+C2H4 7.12E15 0.00 103497 !analogy with cyc5h8¡=¿c2h2+c3h6. Ea REDUCED by 3.57kcal MCYC5-1N¡=¿IC6D14 5.06E15 0.00 66000 !analogy with cyc5h8¡=¿c5h81-3

MCYC5-1N¡=¿I3C6D13 2.52E15 0.00 84850 !analogy with cpt¡=¿c5h10-1 MCYC5-2N¡=¿NC6D14 2.52E15 0.00 93280 !analogy with cyc5h8¡=¿c5h81-4. Ea REDUCED by 3.57kcal (diff. IN BDE OF VIN AND VINS). A/2 DEG=1 !MCYC5-2N¡=¿CYC5H71J+CH3 1.92E+66 -14.22 128100 !analogy with IC4H8¡=¿C3H5-T+CH3 MCYC5-2N¡=¿IC6D14 2.52E15 0.00 96850 !analogy with cyc5h8¡=¿c5h81-4. A/2 DEG=1 MCYC5-2N¡=¿IC6D24 2.53E15 0.00 66000 !analogy with cyc5h8¡=¿c5h81-3 A/2 DEG=1 MCYC5-3N¡=¿CYC5H71-3+CH3 7.94E15 0.0 68834 !analogy with cc5h10=c4h7-a+ch3 (Trenwith, A.B. Trans Faraday Soc. vol 66 1970) MCYC5-3N¡=¿NC6D14 1.26E15 0.00 96850 !analogy with cyc5h8¡=¿c5h81-4. A/2 DEG=1. A/2 2 PATHWAYS MCYC5-3N¡=¿C6H101-5 1.26E15 0.00 96850 !analogy with cyc5h8¡=¿c5h81-4. A/2 DEG=1. A/2 2 PATHWAYS MCYC5-3N¡=¿IC6D13 5.06E15 0.00 66000 !analogy with cyc5h8¡=¿c5h81-3 A/2 DEG=1 MCYC5-3N¡=¿I3C6D15 2.52E15 0.00 96850 !analogy with cyc5h8¡=¿c5h81-4. A/2 DEG=1 MCYC5-4N¡=¿CYC5H71-4+CH3 1.10E26 -2.61 90400 !analogy with IC4H10¡=¿CH3+IC3H7 9Tsang Chem Ref Data 1990, 19) MCYC5-4N¡=¿NC6D14 5.06E15 0.00 66000 !analogy with cyc5h8¡=¿c5h81-3 A/2 2 PATHWAYS MCYC5-4N¡=¿IC6D14 5.04E15 0.00 96850 !ANALOGY WITH CYC5H8¡=¿C5H81-4

! ******* CLASS 9 - CYCLIC C6H9=¿C6H8=¿C6H7=¿C6H6******* ! !Adopted by Dayma et al. MCYC51N3J+O2=mcp2d+HO2 1.580e+12 0.0 1.520e+04 ! Battin-Leclerc, Prog.Energy Combust.Sci. 34(2008)440-498 (alk-alk sec) mcp2d+H¡=¿MCYC51N3J 4.00E+13 0.00 1300 MCYC52N4J+O2=mcp2d+HO2 1.580e+12 0.0 1.520e+04 ! Battin-Leclerc, Prog.Energy Combust.Sci. 34(2008)440-498 (alk-alk sec) mcp2d+H¡=¿MCYC52N4J 4.00E+13 0.00 1300 MCYC52N6J+O2=mcp2d+HO2 1.580e+12 0.0 1.520e+04 ! Battin-Leclerc, Prog.Energy Combust.Sci. 34(2008)440-498 (alk-alk sec) mcp2d+H¡=¿MCYC52N6J 4.00E+13 0.00 1300 MCYC54N3J+O2=mcp2d+HO2 1.580e+12 0.0 1.520e+04 ! Battin-Leclerc, Prog.Energy Combust.Sci. 34(2008)440-498 (alk-alk sec) mcp2d+H¡=¿MCYC54N3J 4.00E+13 0.00 1300 MCYC51N3J=C2H4+C4H5-I 4.000e+13 0.0 3.540e+04 C5H6+CH3=MCYC54N3J 6.300e+10 0.0 7490.0 MCYC51N3J+O2=CH2CO+C3H6CHO-1 1.700E+09 1.0 26400.0 C5H5+CH3=MCYC5-13N 3.058E+105 -27.054 47958.8 MCYC51N3J=I3C6D13-6 2.80E+06 2.10 31013 MCYC54N3J(+M) = C6H96-24 (+M) 7.59E+12 0.15 32940.5 !Ref to CH3cC5H9 LOW / 1.10E-36 16.19 -602.5 / TROE / -21.60 225 28 50000.0 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ C6H95-24 = C6H96-24 3.56E10 0.88 38700 !Matheu et al. C3H5-S + C3H4-P = C6H95-24 8.5E+10 0 7800 !Matheu et al. 2003 mcp2d=mcp2dp+H 9.330E+109 -29.662 135089.9 !Sharma et al., J.Phys.Chem.A, 113(2009)8871-8882 1atm mcp2d=mcp2dt+H 1.735E+97 -24.378 116145.9 !Sharma et al., J.Phys.Chem.A, 113(2009)8871-8882 1atm mcp2d+H=mcp2dp+H2 2.900E+07 2.0 7700.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+H=mcp2dt+H2 1.700E+05 2.5 2480.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+CH3=mcp2dp+CH4 0.750E-07 6.0 5800.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+CH3=mcp2dt+CH4 0.900E-01 4.0 0.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+C5H5=mcp2dp+C5H6 8.000E+01

3.3 19840.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+C5H5=mcp2dt+C5H6
1.600E+12 0.0 15100.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+OH=mcp2dp+H2O
2.700E+06 2.0 450.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+OH=mcp2dt+H2O
1.300E+06 2.0 -2700.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2dt=mcp2dp 3.000E+12
0.0 50400.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 FULVENE+H=mcp2dt 2.600E+13
0.0 1560.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2dp=FULVENE+H 3.160E+13
0.0 34780.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2d+H=C5H6+CH3 1.000E+13
0.0 1300.0 !Herbinet et al., J.Phys.Chem.A, 120(2016)668-682 mcp2dp+O2=FULVENE+HO2 7.500e+10
0.0 2.500e+03 ! Battin-Leclerc, Prog.Energy Combust.Sci., 34(2008)440-498 (alk-all ter) mcp2dt+O2=FULVENE+H
6.900e+11 0.0 1.520e+04 ! Battin-Leclerc, Prog.Energy Combust.Sci., 34(2008)440-498 (all-alk
prim)

END

Appendix B

Relevant publications during PhD

Several parts of this thesis have been published, others are in preparation, and key results have been presented at the conference listed below.

Astrochemistry studies

1. Shock-induced evolution: tracing the fate of coronene in astrophysical environments.

Authors**: D.K. Singh**, L. Biennier, A. Simon, S. Chakraborty, E. Dartois, R. Georges, S. Kassi, V. Chandrasekaran, H. Sabbah, C. Joblin, S. Ranjan, S. Suwas, G. Jagadeesh, and E. Arunan. *Accepted: Astronomy & Astrophysics (A&A) journal.* [203]

Combustion studies

1. Kinetics of the unimolecular decomposition and isomerization of monoalkylated cyclopentane: Ignition delay and thermal decomposition of the monoalkylated cyclopentane: methyl cyclopentane and ethyl cyclopentane. Authors: **Deepak Kumar Singh**, Subharaj Hossain, Shashank Sahu, Chaitanya Sunil Bhoir, Gopalan Jagadeesh, and Elangannan Arunan. *To be submitted*.

2. Unimolecular decomposition of hydrindane in a single pulse shock tube: Experiment and modelling. Authors: **Deepak Kumar Singh**, Subharaj Hossain, Chaitanya Sunil Bhoir, Gopalan Jagadeesh, and Elangannan Arunan. *To be submitted.*

Conference proceedings:

1. Unimolecular Decomposition of trans-Hydrindane in a Single Pulse Shock Tube.

Authors: **DK Singh**, C Bhoir**,** J Gopalan, and E Arunan. Proceedings of the 34th International Symposium on Shock Waves.

Conference Presentations:

1. Poster presentation: Shock-processing of coronene ($C_{24}H_{12}$): insights from real-time optical emission diagnostics. 8th National Symposium on Shock Waves (NSSW-2024), at Indian Institute of Technology Kanpur, India. 12-15, November 2024

2. Poster presentation: Laboratory investigation of shock-induced dissociation of dust analogues: time-resolved broadband emission spectroscopy (TR-BES) studies of C_{60}, C_{70} pyrolysis in shock tube. The International Conference on Molecular Energy Transfer in Complex Systems (iCOMET) was held in Jaipur, India. 12-17, November 2023

3. Poster presentation: Unimolecular decomposition of trans-hydrindane in a single pulse shock tube. 34th International Symposium on Shock Waves (ISSW34) in Daegu, Korea. 16 -21, July 2023

4. Oral presentation: Pyrolysis study of methyl cyclopentane at high temperature and pressure in a single pulse shock tube. 7th National Symposium

on Shock Waves (NSSW-2023) at Physical Research Laboratory (PRL) - Ahmedabad, Gujarat, India. 15-17, February 2023

5. Oral presentation: Temperature calibration of a single pulse shock tube at low pressures using unimolecular decomposition of cyclohexene. International Shock Interaction Symposium 2022, in the Indian Institute of Technology Madras, Chennai, India. 17-20, October 2022

6. Poster presentation: Thermal decomposition study of trans-hydrindane in the single pulse shock tube. 26^{th} International Symposium on Gas Kinetics and Related Phenomena – GK 2022 Rennes, France. 28-31, Aug 2022

Appendix C

Uncertainty analysis

All measured quantities have inherent errors that accumulate throughout the acquisition and calculation process. The intrinsic constraints of instruments concerning accuracy and precision in measuring quantities, along with the propagation of mistakes in derived values, make uncertainty unavoidable in experimental methods. Consequently, they all contribute to the aggregate uncertainty.

The overall uncertainty in the measured values can be expressed in relation to the contributing uncertainty parameters, as delineated in the equation:

$$(\Delta y)^2 = \sum_i \left(\frac{\partial y}{\partial x_i} \Delta x_i \right)^2$$

Where,Δy is the uncertainty in the measured value, Δx is the standard uncertainty in the error source x, and i=1...n is the different source of errors.

Experiments were carried out with precision, and the resultant data have been verified by replicating the technique in order to ensure statistical reliability. All experiments are performed at least five times, and the results are shown with the standard deviation from the mean. In the subsequent discussions, the

uncertainty in the measurement of individual quantities is expressed as $\pm\Delta\%$ relative to the measured values.

Two major sources of error in the Chemical Shock tube facilities are mentioned here:

1. **Facility uncertainty**

- **Initial conditions:** Driver pressure P4, driven pressure P1, and fill composition. ($\pm$0.5% for piezoelectric sensors).
- **Diaphragm burst variability:** The actual burst pressure deviates from the theoretical value, resulting in run-to-run variation in shock speed. (u_s $\pm$0.5%).
- **Incident Shock speed measurement:** Typical uncertainty: $\pm$2%.

If we consider all three, we have a $\pm$2% uncertainty here.

2. **Temperature uncertainty**

Temperature calibration in the shock tube facility. This is reported in detail in Chapter 2 of Chemical Thermometry, section 2.4. Once the incident/reflected shock speed is known, $\mathbf{T}_2$**,** $\mathbf{P}_2$ (incident), and $\mathbf{T}_5$**,** $\mathbf{P}_5$ (reflected) are computed using ideal-gas shock relations. and then a correlation is developed based on previous experimental data in the same temperature ranges. For MST experiments, temperatures are calculated using emission spectroscopy methods, which are detailed in Section .

For our experiments in the CST and MST facility, we have used different instrumentation. Some uncertainty, errors, and instrument calibration are reported in various sections of the chapter where the technique/diagnostics are discussed in detail.

1. **GC uncertainty and calibration methods have been reported in Chapters 04 and 05**. These calculations and details are provided in the GC instrumentation section of Chapter 02 2.2.4. For more details on GC calibration, refer to Hossain et al. [130].

2. **Kinetic calculation errors:** The estimated uncertainty in the rate coefficients derived from this study is ±20%. This estimation is based on the calculated activation energy barriers at the level of theory and the standard uncertainties related to the TST and VTST under high-pressure conditions. [262, 130].

3. **Emission spectroscopy and spectrometer calibration** The spectrometer calibration and error details are provided in Chapter 03. 3.3.2.

    - Detector dark noise, thermal noise.
    - Wavelength calibration (±0.1 nm from slits).
    - Intensity calibration (halogen lamp spectral details).
    - C_2 fits calibration.
    - Emissivity data (for soot temperatures/blackbody contribution).

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